



Quantum integrable systems. Quantitative methods in biology

Systèmes intégrables quantiques. Méthodes quantitatives en biologie

Mémoire d'habilitation à diriger les recherches présenté par

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Abstract. Quantum integrable systems have very strong mathematical properties that allow an exact description of their energetic spectrum. From the Bethe equations, I formulate the Baxter “T-Q” relation, that is the starting point of two complementary approaches based on nonlinear integral equations. The first one is known as thermodynamic Bethe ansatz, the second one as Klümper-Batchelor-Pearce-Destri-de Vega. I show the steps toward the derivation of the equations for some of the models concerned. I study the infrared and ultraviolet limits and discuss the numerical approach. Higher rank integrals of motion can be obtained, so gaining some control on the eigenvectors. After, I discuss the Hubbard model in relation to the $N = 4$ supersymmetric gauge theory. The Hubbard model describes hopping electrons on a lattice.

In the second part, I present an evolutionary model based on Turing machines. The goal is to describe aspects of the real biological evolution, or Darwinism, by letting evolve populations of algorithms. Particularly, with this model one can study the mutual transformation of coding/non coding parts in a genome or the presence of an error threshold.

The assembly of oligomeric proteins is an important phenomenon which interests the majority of proteins in a cell. I participated to the creation of the project “Gemini” which has for purpose the investigation of the structural data of the interfaces of such proteins. The objective is to differentiate the role of amino acids and determine the presence of patterns characterizing certain geometries.

Résumé. Les systèmes intégrables quantiques ont des propriétés mathématiques qui permettent la détermination exacte de leur spectre énergétique. A partir des équations de Bethe, je présente la relation de Baxter «T-Q». Celle-ci est à l’origine des deux approches que j’ai prioritairement employé dans mes recherches, les deux basés sur des équations intégrales non linéaires, celui de l’ansatz de Bethe thermodynamique et celui des équations de Klümper-Batchelor-Pearce-Destri-de Vega. Je montre le chemin qui permet de dériver les équations à partir de certain modèles sur réseau. J’évalue les limites infrarouge et ultraviolet et je discute l’approche numérique. D’autres constantes de mouvement peuvent être établies, ce qui permet un certain contrôle sur les vecteurs propres. Enfin, le modèle d’Hubbard, qui décrit des électrons interagissants sur un réseau, est présenté en relation à la théorie de jauge supersymétrique $N = 4$.

Dans la deuxième partie, je présente un modèle d’évolution darwinienne basé sur les machines de Turing. En faisant évoluer une population d’algorithmes, je peut décrire certains aspects de l’évolution biologique, notamment la transformation entre parties codantes et non-codantes dans un génome ou la présence d’un seuil d’erreur.

L’assemblage des protéines oligomériques est un aspect important qui intéresse la majorité des protéines dans une cellule. Le projet «Gemini» que j’ai contribué à créer a pour finalité d’explorer les données structuraux des interfaces des dites protéines pour différencier le rôle des acides aminés et déterminer la présence de patterns typiques de certaines géométries.

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Preface

The text that I present in the next pages aims at giving some flavour of the researches I have carried on after my degree in physics, obtained in 1995. I tried to give to these notes the style of a comprehensible presentation of the ideas that have animated my researches, with emphasis on the unity of the development. The single steps are here presented in a correlated view. The calculation details are usually available on my original papers, therefore they have been omitted here considering space and time constraints too.

For many years, I have been interested in quantum integrable systems. They are physical models with very special properties that allow to evaluate observable quantities with exact calculations. Indeed, exact calculations are seldom possible in theoretical physics. For this reason, it is instructive to be able to perform exact evaluations in some specific model. B. Sutherland entitles “Beautiful models” his book [15] to express the elegant physical and mathematical properties of integrable models. Thus, in the Introduction to Part I, I define and present, in a few examples, a number of basic properties of quantum integrable systems. These examples will be used in the following three chapters. I will describe the work I did on Destri-de Vega equations, in the first chapter, on the thermodynamic Bethe ansatz in the second one, on the Hubbard model in the third one. In each chapter I also give one or few proposals for the future, to show that the respective field is an active domain of research. Of course, I had to make a choice of the subjects I presented and, forcedly, others were excluded to keep the text into a readable size. Particularly, I regret I could mention very little of the physical combinatorics of TBA quasi-particles, work that I have carried on with P. Pearce and that would have required several additional pages.

Around 2006, I started to follow lectures and seminars delivered by people that, coming from a theoretical physicist background, were starting to work on genome, proteins and cells. Two colleagues of my laboratory, L. Frappat and P. Sorba, were working on a quantum group model for the genetic code. I was curious: how can someone even think to apply quantum groups or let say integrable systems, to the genetic code? Now I know that beyond the application of the apparatus of theoretical physics to biology, it is important to find the new ideas, the new equations, the new models that are needed to better capture the properties of biological systems. In the Part II of this text I will clarify this attitude, especially with the motivations at page 81. After a series of lectures by M. Caselle, I started to experiment with an evolutionary model based on Turing machines. The model, created by a colleague of mine, F. Musso, and myself, will be presented in Chapter 5. Near the end of 2007, Paul Sorba was contacted by a biologist interested in finding theoretical physicists for collaboration. This was an unusual request so Paul organized a meeting with C. Lesieur, to listen to her researches and projects. I immediately accepted to participate and the team “Gemini” was created. A few months later a regular collaboration was on, especially after my primitive but successful attempts to use the art of computer programming to search for the protein interfaces. The two projects on biophysics are now my main research activities, and the time I dedicate to integrable systems has been considerably reduced.

I think the changes I made in my activities reflect more than a personal event and highlight the new horizons theoretical physics is called to explore.

Part I

Integrable models

Chapter 1

Introduction

The study of integrable models is the study of physical systems that are too elegant to be true but too physical to be useless.

Take water in a shallow canal (ϕ is the wave amplitude) and you will find the known example of the Korteweg-de Vries equation (KdV, formalized in 1895 but the first observation of solitary waves in a canal dates to 1844 by J. Scott-Russel)

$$\partial_t \phi + \partial_x^3 \phi + 6\phi \partial_x \phi = 0. \quad (1.1)$$

This equation is nonlinear thus different waves are expected to interact each other. Its speciality is that it admits “solitonic” solutions, namely wave packets in which each component emerges undistorted after a scattering event. This rare property is similar to free waves motion, in which different wave components move independently, but is dramatically broken when interactions are switched on, unless there are some special constraints that forbid the distortion. For the sake of precision, notice that the KdV equation has also “normal” dispersive waves. The wave propagation conserves an infinite number of integrals of motion. This makes more clear the presence of the constraints that force the unusual solitonic behaviour. It is a general theorem of Hamiltonian mechanics that if a (classical) system of coordinates q_i, p_i , $i = 1, \dots, N$ and Hamiltonian $H(q, p)$ possesses N independent functions $I_i(q, p)$ such that

$$\{H, I_i\} = 0 = \{I_i, I_j\} \quad (1.2)$$

then there exist N angle-action variables ϕ_i, I_i . The Hamiltonian is a function of the I_i only $H(I_i)$ and the equations of motion can be explicitly solved by just one integration. This is the origin of the name of integrable models.

This theorem is lost when $N \rightarrow \infty$ or for a quantum system, but somehow its “spirit” remains: the presence of several integrals of motion, as is (1.2), over-constraints the scattering parameters of waves or particles and special behaviours appear.

In $1 + 1$ quantum field theory, this has been made precise by showing [2, 1] the absence of particle production and the factorization of the scattering matrix when there are at least two local conserved charges that are integrals of Lorentz tensors of rank two or higher. This theorem has very strong consequences. It implies for example that the scattering is elastic, namely the set of incoming momenta coincides with the set of outgoing momenta. As an example, the factorization is written here for a four particles scattering

$$S_{i_1 \dots i_4}^{j_1 \dots j_4} = \sum_{k_1 k_2 k_3 k_4 l_1 l_2 l_3 l_4} S_{i_1 i_2}^{k_1 k_2} S_{k_1 i_3}^{l_1 l_3} S_{k_2 k_3}^{l_2 l_3} S_{l_1 i_4}^{j_1 k_4} S_{l_2 k_4}^{j_2 l_4} S_{l_3 l_4}^{j_3 j_4} \quad (1.3)$$

but the generalization is simple [2]. The sum goes over internal indices as in Figure 1.1.

The message is clear: an N particles scattering factorizes in $N(N - 1)/2$ two-particle interactions. This means that a scattering event always decomposes into independent two-particle events, without

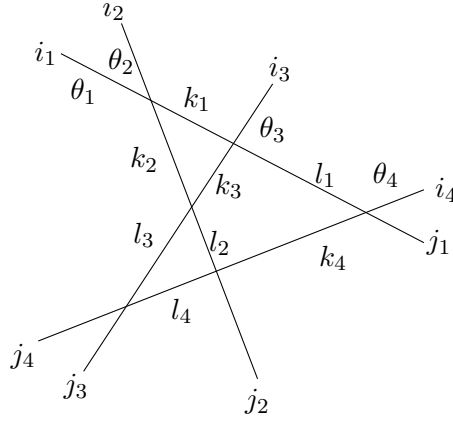


Figure 1.1. A four particles scattering: $i_1 + i_2 + i_3 + i_4 \rightarrow j_1 + j_2 + j_3 + j_4$. Incoming and outgoing momenta do coincide. Time flows downward.

multi-particle effects. Internal indices can only appear when there are particles within the same mass multiplet, otherwise the conservation of momenta forces the conservation of the type of particle $i_1 = k_1 = l_1 = j_1$ and so on. This means that particle annihilation or creation are forbidden outside a mass multiplet.

The factorization comes from the presence of higher rank integrals of motion and from the peculiar property of a two-dimensional plane that non-parallel lines always meet [1]. In a Minkowski space, integrals of motion that are integrals of Lorenz tensors act by parallel shifting trajectories. For example, they parallel shift lines in Figure 1.1. In $1 + 1$ dimensions, two non parallel straight trajectories will always have a cross point but in higher dimensions a parallel movement can suppress the cross point. This geometrical fact indicates that the constraints imposed in higher dimensions are stronger than in $1 + 1$ and the theory will be a free one, as shown by Coleman and Mandula [4]. Therefore, factorization is a very strong property that has no equal in a general field theory. The example of the sine-Gordon model [2] will be presented later, in which the full S-matrix is known.

In order to construct a scattering formalism, we need to use asymptotic states namely we need the so called IN states ($t \rightarrow -\infty$) and OUT states ($t \rightarrow \infty$).

A two-particles scattering then takes the form

$$|A_i(\theta_1)A_j(\theta_2)\rangle_{\text{in}} = \sum_{k,l} S_{ij}^{kl}(\theta_1 - \theta_2) |A_k(\theta_1)A_l(\theta_2)\rangle_{\text{out}} \quad (1.4)$$

where it has been taken into account that Lorentz boosts shift rapidities¹ of a constant amount so the amplitude depends on the difference only.

By parallel shifting lines in Figure 1.1, it is possible to appreciate that there are two possible factorizations for a $3 \rightarrow 3$ particles scattering. Their consistency implies the following equation known as Yang-Baxter equation or factorization equation

$$\sum_{k_1, k_2, k_3} S_{i_1 i_2}^{k_1 k_2}(\theta_1 - \theta_2) S_{k_1 i_3}^{j_1 k_3}(\theta_1 - \theta_3) S_{k_2 k_3}^{j_2 j_3}(\theta_2 - \theta_3) = \sum_{k_1, k_2, k_3} S_{i_2 i_3}^{k_2 k_3}(\theta_2 - \theta_3) S_{i_1 k_3}^{k_1 j_3}(\theta_1 - \theta_3) S_{k_1 k_2}^{j_1 j_2}(\theta_1 - \theta_2) \quad (1.5)$$

This equation characterizes quantum integrability. It first appeared in the lattice case as the star-triangle relation obtained in the context of the Ising and six-vertex models (see for example [9]). In the lattice context, scattering amplitudes are replaced by Boltzmann weights.

A fully general definition of integrable theories is difficult because integrable models are found in a variety of cases and contexts from lattice models to continuum theories, from classical to quantum

¹ $E = m \cosh \theta$, $p = m \sinh \theta$, $\sinh \theta = \frac{v}{\sqrt{1-v^2}}$

dynamics. Therefore, rather than trying to give a general definition, I prefer to indicate the most relevant features. Indeed, the three key ingredients of an integrable theory, both apparent in the KdV and in the sine-Gordon case (see after), are:

- P1 incoming parameters of waves or particles are left unchanged by the scattering event, apart for time shifts,
- P2 there are infinite integrals of motion in involution,
- P3 a Yang-Baxter equation holds.

The first one expresses the conservation of the incoming momenta. The second characterization generalizes the original notion of integrability for classical Hamiltonian systems with finite degrees of freedom. The third property expresses the mathematics of integrability.

1.1 The sine-Gordon model

The sine-Gordon model will be used here as a complete example of several “integrable” ideas. Later it will be used to introduce the nonlinear integral equation of type Klümper-Pearce-Destri-de Vega.

The Lagrangian density is

$$\mathcal{L}[\phi] = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi + \frac{\mu^2}{\beta^2} (\cos \beta \phi - 1) \quad (1.6)$$

and will be considered in 1+1 dimensions (signature of the metric $(1, -1)$). The corresponding equation of motion is

$$\frac{\partial^2 \phi}{\partial t^2} - \frac{\partial^2 \phi}{\partial x^2} = -\frac{\mu^2}{\beta} \sin \beta \phi \quad (1.7)$$

At small β this model appears as a deformation of the Klein-Gordon equation in which μ plays the role of a mass. Expanding the cosinus function in the Lagrangian (or the sinus in the equations of motion) the coupling β first appears with the fourth order term $-\beta \phi^4$, while $\beta = 0$ is precisely the Klein-Gordon equation. The sine-Gordon equation (1.7) admits solitonic solutions, satisfying property P1, that are distinct in three types²

1. the solitons, characterized by $\phi(+\infty, t) - \phi(-\infty, t) = \frac{2\pi}{\beta} m$, $m > 0$, integer;
2. the antisolitons, $\phi(+\infty, t) - \phi(-\infty, t) = \frac{2\pi}{\beta} m$, $m < 0$, integer;
3. the breathers, with $\phi(+\infty, t) = \phi(-\infty, t) = 0$.

Solutions that combine an arbitrary number of these three elementary types do exist and they are all known [3]. They all behave as indicated in property P1. Precisely for this reason, one can think the soliton as an entity “in its own”: it is recognizable and well identified even if it participates to a multicomponent wave.

The name, soliton or antisoliton, suggests that these two waves are distinct because they have opposite sign of the “topological charge”: $\phi(+\infty, t) - \phi(-\infty, t)$. Having the breather zero topological charge, it can be interpreted as a bound state of soliton and antisoliton.

The single soliton state at rest is

$$\phi_s(x) = \frac{4}{\beta} \operatorname{atan} \exp(\mu x) \quad (1.8)$$

²It is usual to interpret as equivalent those fields that differ by multiples of $2\pi/\beta$.

and the single antisoliton is simply given by $\phi_a = -\phi_s$. By Lorentz boost, the single soliton at speed u is $\phi_s((x - ut)/\sqrt{1 - u^2})$

An example of soliton-antisoliton state is given by

$$\phi_{sa}(x, t) = \frac{4}{\beta} \operatorname{atan} \frac{\sinh \frac{\mu ut}{\sqrt{1-u^2}}}{u \cosh \frac{\mu x}{\sqrt{1-u^2}}} \quad (1.9)$$

This state is not the breather (see later). Indeed, at large $|t|$ this state decomposes into a soliton and an antisoliton solution travelling in opposite directions (and non bounded)

$$\begin{aligned} \phi_{sa}(x, t) &\xrightarrow{t \rightarrow -\infty} \phi_s\left(\frac{x + ut}{\sqrt{1 - u^2}} + \log u\right) + \phi_a\left(\frac{x - ut}{\sqrt{1 - u^2}} - \log u\right) \\ \phi_{sa}(x, t) &\xrightarrow{t \rightarrow \infty} \phi_s\left(\frac{x + ut}{\sqrt{1 - u^2}} - \log u\right) + \phi_a\left(\frac{x - ut}{\sqrt{1 - u^2}} + \log u\right) \end{aligned} \quad (1.10)$$

Notice that each wave maintains its initial speed, as indicated by property P1, just experiencing a phase shift of $-2\sqrt{1 - u^2}(\log u)/u > 0$, being $0 \leq u \leq 1$. The phase shift is positive namely the two interacting waves accelerate with respect to their asymptotic motion. This acceleration indicates an attraction, consistently with the idea that solitons and antisolitons have opposite charge.

The simplest breather-like solution

$$\phi_b(x, t) = \frac{4}{\beta} \operatorname{atan} \frac{\sin \frac{\mu ut}{\sqrt{1+u^2}}}{u \cosh \frac{\mu x}{\sqrt{1+u^2}}} \quad (1.11)$$

is a time periodic solution that takes its name from the fact that it resembles a mouth that opens and closes. Curiously, it can be formally obtained from the soliton-antisoliton state (1.9) by rotating to an imaginary speed $u \rightarrow iu$. This type of solution can be interpreted as a bound state of a soliton and an antisoliton because it has zero topological charge and because the soliton and antisoliton can attract each other. It is significantly different from the soliton-antisoliton state because, asymptotically, it does not decompose into two infinitely separated waves as it does the soliton-antisoliton state (1.10).

Finally, the sine-Gordon model admits an infinite number of conserved integrals of motion in involution (property P2).

The sine-Gordon model discussed so far is strictly classical namely the field ϕ is a real function of space and time. Nevertheless, the model can be quantized with fields becoming operators on an Hilbert space leading to a scattering theory of quantum particles. Notice that the various solutions given so far do not survive the limit $\beta \rightarrow 0$ namely they aren't perturbative solutions of the Klein-Gordon equation (see after 1.7). The coupling β is not very important in the classical theory and could be removed by redefinition of the field and the space-time coordinates. On the contrary, in the quantum theory, it will play a true physical role.

In [5],[6],[7] some interesting steps of the quantization procedure are performed. In particular, the need to remove ultraviolet divergences and the existence of a lower bound for the ground state energy lead to observe that outside the range

$$0 \leq \beta^2 \leq 8\pi \quad (1.12)$$

the theory seems not well defined, missing a lower bound for the Hamiltonian. Within the range, the theory describes two particles, charge conjugated, that carry the same name of the classical counterparts, soliton and antisoliton, and other particles, corresponding to the breathers.

Within this interval, the theory shows up to coincide with the massive Thirring model, in the sector of even number of solitons plus antisolitons ("even sector"):

$$\mathcal{L}[\psi] = \bar{\psi} i \gamma_\mu \partial^\mu \psi - m_F \bar{\psi} \psi - \frac{1}{2} g j_\mu j^\mu, \quad \text{with} \quad j_\mu = \bar{\psi} \gamma_\mu \psi \quad (1.13)$$

The equivalence of the two models is better stated by saying that they have the same correlation functions in the even sector, provided the respective coupling constants are identified by

$$\frac{\beta^2}{4\pi} = \frac{1}{1 + g/\pi} \quad (1.14)$$

Another useful coupling will be

$$\gamma = \frac{\beta^2}{1 - \frac{\beta^2}{8\pi}} \quad (1.15)$$

Notice that there is no equivalence outside the even sector because the soliton does not correspond to the fermion [10]: the transformation between the two is highly nonlocal. In other words, there are states of sine-Gordon that do not exist in Thirring and vice versa.

The relation between the Thirring and sine-Gordon couplings reveals that the special point $g = 0$ or $\beta^2 = 4\pi$ describes a free massive Dirac theory. This free point separates two distinct regimes

$$\begin{array}{llll} \text{repulsive} & -\frac{\pi}{2} < g < 0 & 8\pi > \beta^2 > 4\pi & \infty > \gamma > 8\pi \\ \text{attractive} & 0 < g < \infty & 4\pi > \beta^2 > 0 & 8\pi > \gamma > 0 \end{array} \quad (1.16)$$

The repulsive regime is so called because no bound state of the Thirring fermions or sine-Gordon bosons is observed. Vice versa, in the attractive regime the quantum fields corresponding to the classical breathers describe bound states between solitons and antisolitons. The attractive regime admits small values of beta, where the theory is close to a ϕ^4 theory (1.6) but with an unusual attractive sign

$$\mathcal{L}[\phi] = \frac{1}{2} \partial_\mu \phi \partial^\mu \phi - \frac{\mu^2}{2} \phi^2 + \frac{\mu^2}{4!} \beta^2 \phi^4 \dots \quad (1.17)$$

The mass of the breathers is given by the exact expression

$$M_n = 2M \sin \frac{n\gamma}{16}, \quad n = 1, 2, \dots, < \frac{8\pi}{\gamma}, \quad (1.18)$$

where M is the mass of the soliton. In the repulsive regime, no integer is in the range, indicating that breathers do not exist; this mass formula makes sense in the attractive regime only. The interpretation of breathers as bound states comes also from the fact that the breather masses are below the threshold $M_n < 2M$. These breathers originate in the quantization of the classical breather solutions and, from (1.17), they correspond to the perturbation of the Klein-Gordon particles. Indeed, given that the soliton mass at leading order is

$$M = \frac{8\mu}{\gamma} \quad (1.19)$$

the smallest breather mass M_1 for in the weak coupling $\beta^2 \rightarrow 0$ is

$$M_1 = 2 \frac{8\mu}{\gamma} \frac{\gamma}{16} = \mu \quad (1.20)$$

So, the lowest breather originates in the perturbation of the Klein-Gordon boson. Notice that the breather is a bound state while the Klein-Gordon model has no bound states at all. This is true even for the n th breather

$$M_n = n\mu \quad (1.21)$$

so the Klein-Gordon free multiparticle states become bound states in sine-Gordon. Differently from the breather, the soliton doesn't emerge from the Klein-Gordon theory: its mass diverges in this limit (1.19) so this particle is considered decoupled from the theory.

The relations (1.14, 1.16) indicate a strong/weak duality between sine-Gordon and Thirring: strong interactions in one model correspond to weak interactions in the other. Can we see a physical track of

this? Yes, for example in the weak sine-Gordon regime $\beta^2 \rightarrow 0$. Indeed, the n th breather appears to be a bound state of n Klein-Gordon particles (1.21). It is a stable state that takes its stability from the strong fermionic coupling $g \gg 0$ of Thirring. Moving to higher values of β^2 , the fermionic coupling decreases therefore we expect to have less and less stable breathers, consistently with the mass expression (1.18). In the same weak regime $\beta^2 \rightarrow 0$, the soliton is decoupled from the theory as it has an almost infinite mass (1.19). It is strongly coupled in the repulsive regime where its mass is small.

The most important feature is that the quantum sine-Gordon model is still integrable. This was first seen by showing that conservation laws do survive perturbative quantization. Now this result is known beyond perturbation theory [8] and grants the already discussed necessary conditions for the factorization of scattering (1.3). Thus, all the properties P1, P2, P3 hold.

Particle annihilation and creation are forbidden. Consequently, all the bound states in (1.18) are stable particles even when there are breather states above the creation threshold $M_n > 2M_1$. This happens for some n and for sufficiently small γ . Notice that in the attractive regime the lowest breather is always the lightest particle. Moving toward the repulsive regime, one observes that the n th breather disappears into a soliton-antisoliton state when $8\pi/\gamma$ is a positive integer

$$\lim_{\gamma \rightarrow (\frac{8\pi}{n})^-} M_n = 2M \quad (1.22)$$

The lowest breather disappears at the free fermion point $\gamma = 8\pi$.

If one can show the existence of conserved charges as required in the factorization theorem, the two particles scattering amplitudes can be evaluated on the basis of their symmetries. In other words, the Yang-Baxter equation (1.5) supplemented with usual analytic properties (poles from mass spectrum), unitarity and crossing symmetry, is (often) enough to find the scattering amplitudes. This avoids a much more lengthy calculation based on the evaluation of Feynman diagrams to all orders. For the sine-Gordon model, this has been done in [2].

The notation in (1.4) is now used to write down the amplitudes. For the solitonic part only, there are three $2 \rightarrow 2$ particle processes

$$\begin{aligned} A_s + A_s &\rightarrow A_s + A_s \\ A_s + A_{\bar{s}} &\rightarrow A_s + A_{\bar{s}} \\ A_{\bar{s}} + A_{\bar{s}} &\rightarrow A_{\bar{s}} + A_{\bar{s}} \end{aligned} \quad (1.23)$$

where A_s ($A_{\bar{s}}$) indicates a soliton (antisoliton) momentum state. Charge conjugation symmetry makes the first and the last processes to have identical amplitude. Using $\theta = \theta_1 - \theta_2$, we have

$$\begin{aligned} |A_s(\theta_1)A_s(\theta_2)\rangle_{\text{in}} &= S(\theta) |A_s(\theta_1)A_s(\theta_2)\rangle_{\text{out}} \\ |A_s(\theta_1)A_{\bar{s}}(\theta_2)\rangle_{\text{in}} &= S_T(\theta) |A_s(\theta_1)A_{\bar{s}}(\theta_2)\rangle_{\text{out}} + S_R(\theta) |A_{\bar{s}}(\theta_1)A_s(\theta_2)\rangle_{\text{out}} \\ |A_{\bar{s}}(\theta_1)A_{\bar{s}}(\theta_2)\rangle_{\text{in}} &= S(\theta) |A_{\bar{s}}(\theta_1)A_{\bar{s}}(\theta_2)\rangle_{\text{out}} \end{aligned} \quad (1.24)$$

There are just three independent amplitudes to be determined, that we organize in a 4×4 matrix to be used in the Yang-Baxter equation (1.5)

$$S = \begin{pmatrix} S(\theta) & & & \\ & S_T(\theta) & S_R(\theta) & \\ & S_R(\theta) & S_T(\theta) & \\ & & & S(\theta) \end{pmatrix} \quad (1.25)$$

Notice that, in the Yang-Baxter equation, the conservation of the set of momenta forbids amplitudes describing particles with different mass to mix each other. In sine-Gordon, there are just two particles with identical mass, the soliton and the antisoliton, with interactions listed in (1.23). This means that the

scattering processes involving a breather do not mix with those in (1.23). As the breathers have different mass, the following processes are of pure transmission, reflection being forbidden

$$\begin{aligned} A_s + B_n &\rightarrow A_s + B_n \\ A_{\bar{s}} + B_n &\rightarrow A_{\bar{s}} + B_n \\ B_m + B_n &\rightarrow B_m + B_n \end{aligned} \quad (1.26)$$

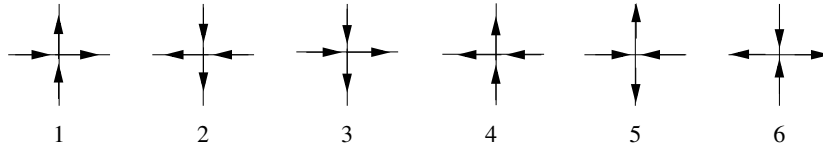
The whole knowledge of the scattering amplitudes is not needed. The soliton part is given by

$$S = \begin{pmatrix} -i \sinh\left(\frac{8\pi}{\gamma}(i\pi - \theta)\right) & & & & & \\ & -i \sinh\left(\frac{8\pi}{\gamma}\theta\right) & \sin\frac{8\pi^2}{\gamma} & & & \\ & \sin\frac{8\pi^2}{\gamma} & -i \sinh\left(\frac{8\pi}{\gamma}\theta\right) & & & \\ & & & -i \sinh\left(\frac{8\pi}{\gamma}(i\pi - \theta)\right) & & \\ & & & & -i \sinh\left(\frac{8\pi}{\gamma}(i\pi - \theta)\right) & \\ & & & & & -i \sinh\left(\frac{8\pi}{\gamma}(i\pi - \theta)\right) \end{pmatrix} U(\theta) \quad (1.27)$$

where $U(\theta)$ is a known factor. The expression of the scattering matrix will be useful soon, in relation to the six-vertex model.

1.2 The six-vertex model

It is a two dimensional classical statistical mechanics model in which interactions are associated with a vertex: the four bonds surrounding a vertex fix the Boltzmann weight associated with it. In the present model the possible vertices are those shown here:



A bond can therefore be in either one of two states, that will be indicated by “0” or “1” (0 associated to up and right, 1 associated to down and left). Initially, this model was introduced as a two dimensional idealization of an ice crystal and called ice-type model. Indeed, the vertex represents the oxygen atom and the four bonds connected to it represent two covalent bonds and two hydrogen bonds. The arrows indicate to which oxygen the hydrogen atom is closer, thus differentiating the covalent bonds from the hydrogen bonds.

The Boltzmann weights for a vertex are nonnegative values indicated by $w_1, w_2, w_3, w_4, w_5, w_6$. Hereafter I will put $w_1 = w_2 = a, w_3 = w_4 = b$ and $w_5 = w_6 = c$, as in [9]. Their product on the whole lattice vertices is summed on all the configurations to build up the partition function

$$\mathcal{Z} = \sum_{\text{conf}} w_1^{N_1} w_2^{N_2} w_3^{N_3} w_4^{N_4} w_5^{N_5} w_6^{N_6} \quad (1.28)$$

where N_i is the number of occurrences of the type i vertex in the lattice. Periodic boundary conditions will now be used in the vertical and horizontal directions. The expression for the partition function takes a useful form if one introduces the transfer matrix and the so called R matrix. The transfer matrix \mathbf{T} is a $2^N \times 2^N$ matrix that describes how the system “evolves” from a row to the next one of the lattice. The R matrix somehow summarizes the possible behaviours on a single vertex or lattice site. On a given row, the vertical bond at site i is associated with a local vector space $V_i = \mathbb{C}^2$. Also, A represents an auxiliary

space $A = \mathbb{C}^2$. The R matrix is a 4×4 matrix acting on $A \otimes V_i$ (or else on $A \otimes A$)

$$R = \begin{pmatrix} a & & & \\ & b & c & \\ & c & b & \\ & & & a \end{pmatrix} \quad (1.29)$$

00 01 10 11

where the lower line indicates how the entries are interpreted with respect to the two possible bond configurations. The transfer matrix acts on the physical vector space \mathcal{V} and is a product of R matrices

$$\begin{aligned} \mathcal{V} &= V_1 \otimes V_2 \otimes \dots \otimes V_N \\ \mathbf{T} : \mathcal{V} &\rightarrow \mathcal{V} \\ \mathbf{T} &= \text{Tr}_A R_{A1} R_{A2} \dots R_{AN} \end{aligned} \quad (1.30)$$

where the trace is taken on the auxiliary space A^3 . The partition function can be written as the trace of the product of M transfer matrices (if M is the number of rows of the lattice)

$$\mathcal{Z} = \text{Tr} \mathbf{T}^M \quad (1.31)$$

having now taken the trace on \mathcal{V} , namely on all the horizontal sites. It turns out that if the Boltzmann weights have an appropriate form, the transfer matrix generates an integrable system. The following parametrization makes the game

$$a = a(\theta) = \sinh \frac{\gamma_{6v}}{\pi}(\theta + i\pi), \quad b = b(\theta) = \sinh \frac{\gamma_{6v}}{\pi}\theta, \quad c = c(\theta) = i \sin \gamma_{6v} \quad (1.32)$$

and gives an R matrix function of the spectral parameter⁴ θ , $R(\theta)$, and also of the coupling γ_{6v} . The R matrix satisfies a Yang-Baxter equation (see later).

It turns out that this parametrization is very much the same as in (1.27), except for the identification of the couplings that requires some care and will be done later. This means that the integrable sine-Gordon model and the six-vertex model have something in common. Anticipating a later discussion, one can use the six-vertex model for a lattice regularization of the sine-Gordon. In other words, sine-Gordon appears as a certain continuum limit of the six-vertex model, provided a mass scale is introduced.

The disadvantage of the parametrization (1.32) is that it introduces complex Boltzmann weights and this looks odd in statistical mechanics. However, this is not a serious problem, first because the statements that concern integrability do hold for arbitrary complex parameters, second because it is easy to get a real transfer matrix, simply by using an imaginary value for θ .

The Yang-Baxter equation satisfied by the R matrix (1.32) is

$$R_{12}(\lambda - \mu) R_{13}(\lambda) R_{23}(\mu) = R_{23}(\mu) R_{13}(\lambda) R_{12}(\lambda - \mu) \quad (1.33)$$

where λ, μ are arbitrary complex spectral parameters. Thus, property P3 above also holds for the lattice case. From this equation, a very general construction shows that the transfer matrix forms a commuting family

$$[\mathbf{T}(\theta), \mathbf{T}(\theta')] = 0 \quad (1.34)$$

³Here, the standard notation of lattice integrable systems is used such that the lower indices of the matrix do not indicate its entries but the spaces on which the matrix acts (namely the auxiliary space and one of the horizontal lattice sites, enumerated from 1 to N).

⁴The spectral parameter is a complex number that is used to describe a sort of off-shell physics; usually it is fixed to a specific value or interval to construct a physical model.

	XXZ	six-vertex
$\Delta > 1$	ferromagnetic	ferroelectric, vertex: one of 1,2,3,4
$-1 < \Delta < 1$	critical case, multi-degenerate ground state	
$\Delta < -1$	antiferromagnetic	antiferroelectric, vertices 5 and 6 alternate

Table 1.1. The thermodynamic phases of the XXZ and six-vertex model are indicated. The XXZ model being defined by the Hamiltonian, the phases are understood at zero temperature, while the six-vertex phases are read from the transfer matrix and contain a temperature, hidden in the parameters a, b, c . Moreover, one-dimensional models do not break symmetries: phase transitions can only occur at zero temperature.

for arbitrary values of the spectral parameters. Now, any expansion of the transfer matrix produces commuting objects. In particular, it is possible to evaluate the logarithmic derivative of the transfer matrix

$$H = \mathcal{A} \left. \frac{d \log \mathbf{T}(\theta)}{d\theta} \right|_{\frac{i\pi}{2}} \quad (1.35)$$

and all the higher derivatives. The operators obtained with this procedure are local and commutative therefore we conclude that property P2 is satisfied for the lattice model. The logarithmic derivative is manageable, at least for the six-vertex model, and leads to a very interesting expression (the overall factor \mathcal{A} is easy to evaluate but not very important)

$$\begin{aligned} H &= - \sum_{i=1}^{N-1} \left[\sigma_i^1 \sigma_{i+1}^1 + \sigma_i^2 \sigma_{i+1}^2 + \Delta (1 + \sigma_i^3 \sigma_{i+1}^3) \right] \\ \Delta &= \cos \gamma_{6v} \end{aligned} \quad (1.36)$$

The σ_i^j , $j = 1, 2, 3$ are Pauli matrices acting on the site i , where, by definition, different site matrices always commute. This one-dimensional lattice quantum Hamiltonian is known as XXZ model. The more general version with three different coefficients and three spatial dimensions was introduced by W. Heisenberg (1928) as a natural physical description of magnetism in solid state physics. Indeed, the Heisenberg idea was to consider, on each lattice site, a quantum magnetic needle of spin $\frac{1}{2}$ fully free to rotate. The magnetic needle is assumed sensitive to the nearest neighbor needles with the simplest possible coupling of magnetic dipoles. At $\gamma_{6v} = 0$ it is fully isotropic with rotational $su(2)$ symmetry. As soon as $\gamma_{6v} \neq 0$ is introduced, the model acquires an anisotropy.

The XXX Hamiltonian is free of couplings apart from the overall sign. Given the present sign choice, it is apparent that adjacent parallel spins lower the energy. This explains the name “ferromagnetic” attributed to the Hamiltonian in (1.36), if $\Delta = 1$. The Hamiltonian with opposite sign is known as “antiferromagnetic”.

The presence of $\Delta \neq 1$ in the XXZ model spoils this distinction because the ferromagnetic or antiferromagnetic behavior depends by the coupling and the name cannot be attached to the Hamiltonian itself but to the phases it describes. The phases of the two models are indicated in table 1.1.

Finally, as the XXZ model is embedded in XYZ, the six-vertex is embedded in the more general eight-vertex model, that is still integrable.

The XXZ model is presented in the review [14] and also in the book [15].

1.2.1 The Baxter T-Q relation

The one-dimensional XXZ model has the merit of having inaugurated the studies of quantum integrable systems and of the methods known as Bethe ansatz, in the celebrated Bethe paper [12].

Indeed, his idea was to try to guess, or ansatz, the appropriate eigenfunctions for the Hamiltonian (1.36), from a trial form, then show that the guess is correct. This approach is called coordinate Bethe ansatz and produces a set of constraints on the parameters of the wave function known as Bethe equations. Baxter [9], from the Bethe equations, was able to show the existence of a T-Q relation (3.6) for the transfer matrix. After, he could reverse the approach and, with a more direct construction, he derived the T-Q relation from the Yang-Baxter equation. Therefore, he obtained the Bethe equations from the T-Q relation. The presentation will follow the second approach.

Following Baxter, the transfer matrix satisfies a functional equation [9] for periodic boundary conditions on a row of N sites. This means that there exist a matrix $Q(u)$ such that

$$T(u)Q(u) = f\left(u + \frac{\lambda}{2}\right) Q(u - \lambda) + f\left(u - \frac{\lambda}{2}\right) Q(u + \lambda) \quad (1.37)$$

where we have used

$$f(u) = \left(\frac{\sin u}{\sin \lambda}\right)^N \quad (1.38)$$

The coupling and spectral parameters are related to the previous ones by

$$\lambda = \gamma_{6v}, \quad u = -i\frac{\gamma_{6v}}{\pi}\theta \quad (1.39)$$

The new operator $Q(u)$ forms a family of matrices that commute each other and with the transfer matrix $[Q(u), Q(v)] = [Q(u), T(v)] = 0$. This implies that the same functional equation (1.37) holds true also for the eigenvalues $T(u)$ and $Q(u)$. Moreover, all these operators have the same eigenvectors independent of u . The eigenvalues of Q are given by

$$Q(u) = \prod_{j=1}^M \sin(u - u_j) \quad (1.40)$$

where u_j are the Bethe roots and appear now as zeros of the eigenvalues of $Q(u)$. The Bethe ansatz equations result by imposing that the transfer matrix eigenvalues on the left are entire functions. Indeed, when $Q(u) = 0$, being $T(u)$ entire, the right hand side must vanish. This forces the constraints (Bethe equations)

$$\left(\frac{\sin\left(u + \frac{\lambda}{2}\right)}{\sin\left(u - \frac{\lambda}{2}\right)}\right)^N = -\frac{Q(u + \lambda)}{Q(u - \lambda)} \quad (1.41)$$

The T-Q relation (1.37) shows that the columns of $Q(u)$ are eigenvectors of T so this equation actually provides both information on eigenvalues and eigenvectors.

The Bethe equations have a finite number of solutions in the periodicity strip

$$\text{Re}(u) \in [0, \pi] \quad (1.42)$$

This is easily seen because they can be transformed into algebraic equations in the new variables

$$z_j = \exp(i u_j)$$

Notice that the lattice model also has a finite number of states: indeed,

$$\dim \mathcal{V} = 2^N$$

This is the size of the transfer matrix and is also the number of expected solutions of the Bethe equations. Indeed, it has been possible to show that the Bethe equations have the correct number of solutions and that the corresponding Bethe eigenvectors form a base for \mathcal{V} , see [22], [23] and references there. This is referred to as the “completeness” of the Bethe ansatz. One feature observed is that Bethe roots satisfy a Pauli-like principle, in the sense that they are all distinct: there is no need to consider solutions with $u_j = u_k$ for different $j \neq k$.

1.3 Conformal field theories

Conformal field theories (CFT) are scale invariant quantum field theories. They were introduced for two main reasons, one being the study of continuum phase transitions and the other being the interest of describing quantum strings on their world sheet, a two-dimensional surface in a ten-dimensional space. This second point strongly motivated the treatment of the two dimensional case, initiated in the fundamental work [16]. Curiously, the subsequent development of the two-dimensional case, instead, was much more statistical mechanics oriented. Two-dimensional conformal field theories are very close to the subject of quantum integrability because they also are integrable theories and, often, they appear in certain limits of lattice or continuum integrable theories. These topics and some connections between conformal field theory and integrability will be discussed later, in relation to several of the investigations that I have carried on: nonlinear Destri-de Vega equations, thermodynamic Bethe ansatz equations and so on.

Four-dimensional conformal field theories are studied in the Maldacena gauge/string duality framework. In particular, the superconformal gauge theory $\mathcal{N} = 4$ appears in relation to some integrable theories, after the work [17]. In particular, in that paper the XXX model appeared. As the paper [16] created the bridge between integrable models and two-dimensional field theories, [17] inaugurated the interchange between (some) aspects of integrable models and four-dimensional superconformal field theories.

In the two-dimensional case, the generators of the conformal symmetry are the modes of the Virasoro algebra (\mathcal{V})

$$[L_m, L_n] = (m - n)L_{m+n} + \frac{c}{12}(m^3 - m)\delta_{m+n,0} \quad (1.43)$$

where the constant c that appears in the central extension term is called *conformal anomaly* or often *central charge*. For a physical theory on the Minkowski plane or on a cylinder geometry in which the space is periodic and the time flows in the infinite direction, the algebra of the full conformal group is the tensor product of two copies of (1.43) $\mathcal{V} \otimes \bar{\mathcal{V}}$. For other geometries, it can be different. For example, on a strip (finite space, infinite time) there is a single copy. According to this, the Hamiltonian is $L_0 + \bar{L}_0$ for the plane or cylinder and is L_0 in a strip. We need this distinction because, later on, we will use both types of space-time. Somehow, the presence of two copies in the plane and in the cylinder with periodic space is justified because there are two types of movers: left and right movers, namely massless particles moving at the speed of light toward left or right⁵. In a strip, corresponding to a finite space with spatial borders, movement is not allowed, thus just one copy remains.

All the states of a CFT must lie in some irreducible representation of the algebra (1.43). Physical representations must have the Hamiltonian spectrum bounded from below, i.e. they must contain a so called *highest weight state* (HWS) $|\Delta\rangle$ for which

$$L_0|\Delta\rangle = \Delta|\Delta\rangle \quad , \quad L_n|\Delta\rangle = 0 \quad , \quad n > 0 \quad (1.44)$$

These representations are known as *highest weight representations* (HWR). The irreducible representations of \mathcal{V} are labelled by two numbers, namely the central charge c and the conformal dimension Δ . We shall denote the HWRs of \mathcal{V} by $\mathcal{V}_c(\Delta)$. For a given theory, the Hilbert space \mathcal{H} of the theory is built up of all possible representations $\mathcal{V}_c(\Delta)$ with the same c , each one with a certain multiplicity:

$$\mathcal{H} = \bigoplus_{\Delta, \bar{\Delta}} \mathcal{N}_{\Delta, \bar{\Delta}} \mathcal{V}_c(\Delta) \otimes \bar{\mathcal{V}}_c(\bar{\Delta}) \quad (1.45)$$

If a certain $\mathcal{V}_c(\Delta) \otimes \bar{\mathcal{V}}_c(\bar{\Delta})$ does not appear, then simply $\mathcal{N}_{\Delta, \bar{\Delta}} = 0$. The numbers $\mathcal{N}_{\Delta, \bar{\Delta}}$ count the multiplicity of each representation in \mathcal{H} , therefore they must always be non negative integers. They

⁵Conformal invariance implies that particles are massless and move at the speed of light.

are not fixed by conformal invariance alone as they depend on the geometry and on possible boundary conditions.

Every HWS (1.44) in the theory can be put in one-to-one correspondence with a field through the formula $|\Delta, \bar{\Delta}\rangle = A_{\Delta, \bar{\Delta}}(0, 0)|0, 0\rangle$, where the vacuum $|0, 0\rangle$ is projective (i.e. $L_0, \bar{L}_0, L_{\pm 1}, \bar{L}_{\pm 1}$) invariant. In particular the HWS (1.44) correspond to some fields $\phi_{\Delta, \bar{\Delta}}(z, \bar{z})$ that transform under the conformal group as

$$\phi_{\Delta, \bar{\Delta}}(z, \bar{z}) = \left(\frac{\partial z'}{\partial z}\right)^{\Delta} \left(\frac{\partial \bar{z}'}{\partial \bar{z}}\right)^{\bar{\Delta}} \phi_{\Delta, \bar{\Delta}}(z', \bar{z}') \quad (1.46)$$

They are called *primary fields*. Non primary fields (secondaries) do have much more involved transformations. A basis for the states can be obtained by applying strings of $L_n, n < 0$ to $|\Delta\rangle$. The commutation relations imply

$$L_0 L_n^k |\Delta\rangle = (\Delta + nk) L_n^k |\Delta\rangle \quad (1.47)$$

Therefore L_0 eigenvalues organize the space $\mathcal{V}_c(\Delta)$ (called a *module*) so that the states lie on a “stair” whose N -th step (called the N -th *level*) has $L_0 = \Delta + N$

states	level	L_0
.....
$L_{-3} \Delta\rangle, L_{-2}L_{-1} \Delta\rangle, L_{-1}^3 \Delta\rangle$	3	$\Delta + 3$
$L_{-2} \Delta\rangle, L_{-1}^2 \Delta\rangle$	2	$\Delta + 2$
$L_{-1} \Delta\rangle$	1	$\Delta + 1$
$ \Delta\rangle$	0	Δ

(1.48)

All the fields corresponding to the HWR $\mathcal{V}_c(\Delta)$ are said to be in the *conformal family* $[\phi_{\Delta}]$ generated by the primary field ϕ_{Δ} .

For the following, the most important conformal models will be those known as minimal models, characterized by the central charge

$$c = 1 - \frac{6}{p(p+1)} \quad (1.49)$$

with $p = 3, 4, \dots$. These models are all unitary and all have a finite number of primary fields. The first one, $c = \frac{1}{2}$, is the universality class of the Ising model. The next one $c = \frac{7}{10}$, is the tricritical Ising model, namely an Ising model with vacancies. After, we find the universality class of the three-states Potts model and so. The limit $p \rightarrow \infty$ is also a CFT; it is one point of the class of the free massless boson with $c = 1$.

Indeed, $c = 1$ is a wide class of unitary conformal field theories, all derived from a free massless boson compactified in the following way

$$\phi \equiv \phi + 2\pi m R, \quad m \in \mathbb{Z} \quad (1.50)$$

and radially quantized. A full description of this theory would be very long. A sketch is presented in [20]. The theory turns out to be characterized by certain vertex operators

$$V_{(n, m)}(z, \bar{z}) =: \exp i(p_+ \phi(z) + p_- \bar{\phi}(\bar{z})) : , \quad p_{\pm} = \frac{n}{R} \pm \frac{1}{2} m R. \quad (1.51)$$

with conformal weight $\Delta = p_+^2/2, \bar{\Delta} = p_-^2/2$.

Each pair (n, m) describes a different sector of the theory; its states are obtained by the action of the modes of the fields, $\partial_z \phi$ and $\bar{\partial}_z \bar{\phi}$, in a standard Fock space construction.

It is important to stress that a particular $c = 1$ CFT is specified by giving the spectrum of the quantum numbers (n, m) (and the compactification radius R) such that the corresponding set of vertex operators (and their descendants) forms a *closed and local* operator algebra. The locality requirement is equivalent

to the fact that the operator product expansions of any two such local operators is single-valued in the complex plane of z .

By this requirement of locality, it was proved in [33] that there are only two maximal local subalgebras of vertex operators: \mathcal{A}_b , purely bosonic, generated by the vertex operators

$$V_{(n,m)} : n, m \in \mathbb{Z} \quad (1.52)$$

and \mathcal{A}_f , fermionic, generated by

$$V_{(n,m)} : n \in \mathbb{Z}, m \in 2\mathbb{Z} \quad \text{or} \quad n \in \mathbb{Z} + \frac{1}{2}, m \in 2\mathbb{Z} + 1. \quad (1.53)$$

Other sets of vertex operators can be built, but the product of two of them gives a nonlocal expression (namely the operator product expansion is multi-valued).

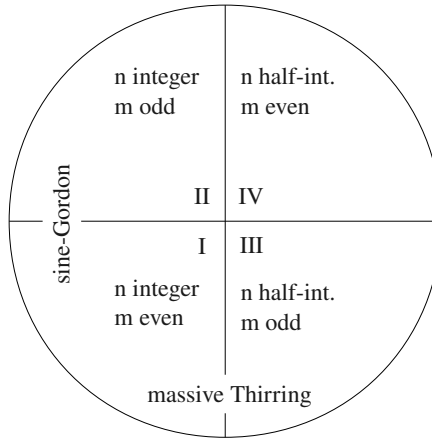


Figure 1.2. The family of vertex operators $V_{(n,m)}$ with $n \in \mathbb{Z}/2$ and $m \in \mathbb{Z}$. Sectors **I** and **II** are \mathcal{A}_b , namely the ultraviolet limit of the sine-Gordon model. Sectors **I** and **III** are \mathcal{A}_f , that defines the UV behaviour of massive Thirring. Sector **I** is the one where sine-Gordon and massive Thirring are equivalent. **IV** is a sector of non mutually local vertex operators.

The sine-Gordon model appears as a integrable perturbation of the $c = 1$ free boson by an operator with scaling dimensions $(\Delta, \bar{\Delta}) = (\beta^2/8\pi, \beta^2/8\pi)$. The corresponding unperturbed algebra is \mathcal{A}_b while the algebra \mathcal{A}_f can be perturbed to give rise to the massive Thirring model. The compactification radius and the sine-Gordon coupling are related by

$$R^2 = \frac{4\pi}{\beta^2}$$

1.4 Perturbed conformal field theory

We may think to define a quantum field theory as a deformation of a conformal field theory by some operators [51], i.e. to perturb the action of a CFT as in the following expression

$$S[\Phi_i] = S_{CFT} + \sum_{i=1}^n \lambda_i \int d^2x \Phi_i(x) \quad (1.54)$$

Of course, the class of two-dimensional field theories is larger than the one described by this action. Nevertheless, this class of *perturbed conformal field theories* has a special role because it describes the

vicinity of critical points in the theory of critical phenomena. The main goal is to be able to compute off-critical correlation functions by

$$\langle X \rangle = \int \mathcal{D}\varphi X e^{-S[\Phi]} = \int \mathcal{D}\varphi X \exp \left[-S_{CFT} - \lambda \int d^2x \Phi(x) \right] \quad (1.55)$$

Indeed, expanding in powers of λ one can express $\langle X \rangle$ as a series of conformal correlators (in principle computable by conformal field theory techniques). The perturbed theory is especially important if it maintains the integrability of the conformal point. If so, the perturbed theory has a factorized scattering.

The possible perturbing fields are classified with respect to their renormalization group action as

- **relevant** if $\Delta < 1$. If such a field perturbs a conformal action, it creates exactly the situation described above, i.e. the theory starts to flow along a renormalization group trajectory going to some IR destiny.
- **irrelevant** if $\Delta > 1$. Such fields correspond to perturbations which describe the neighborhood of non trivial IR fixed points. It is more appropriate to refer to them as *attraction* fields because the perturbation is not able to move off the critical point; it actually always returns to it. We shall not deal with this case in the following, but the interested reader may consult, for example, [18] to see some possible applications of this situation.
- **marginal** if $\Delta = 1$. Their classification requires investigation of derivatives of the beta function.

1.5 Conclusion

A typical phenomenon of integrable systems emerges, namely the fact that different models can transform the one into the other in some conditions and also shown to be equivalent. Firstly, the equivalence of the bosonic sine-Gordon model with the fermionic massive Thirring has been presented. After, the correspondence of the six-vertex model and the XXZ model has been shown. Moreover, these lattice models share the same R or S matrix as the sine-Gordon model. At this point, it is natural to expect that a proper continuum limit on the six-vertex model could produce sine-Gordon; indeed, this is the case and will be discussed later in the context of the nonlinear integral equation. This “game” of models that are related one to the other can be pushed forward. For example, if $\Delta = 0$, the XXZ model reduces to the XX model, that can also be written as a lattice free fermion (one fermionic species). If $\Delta \rightarrow \pm\infty$, one obtains the one-dimensional Ising model. More important for what follows, the XXX model emerges in the high coupling limit of the Hubbard model, that is a lattice quantum model of two fermionic species (namely, spin up, spin down).

The deep reason of these strong connections between different models is that, for a given size of the R matrix, there are very few solutions of the Yang-Baxter equation. In other words, there are very few classes of integrability, classified by the solution of the Yang-Baxter equation.

Chapter 2

A nonlinear equation for the Bethe ansatz

2.1 Light-cone lattice

In this section I present a lattice regularization of the Sine-Gordon model which is particularly suitable to study finite size effects. It is well known to lattice theorists that the same continuum theory can often be obtained as limit of many different lattice theories. This means that there are many possible regularizations of the same theory and it is customary to choose the lattice action possessing the properties that best fit calculational needs. In the present context the main goal is to have a lattice discretization of the Sine-Gordon model that preserves the property of integrability. The following light-cone lattice construction is a way (not the unique!) to achieve this goal.

In two dimensions, the most obvious approach would be to use a rectangular lattice with axes corresponding to space and time directions. Here, a different approach [19] is adopted where space-time is discretized along light-cone directions. Light-cone coordinates in Euclidean or Minkowski space-time are

$$x_+ = x + t, \quad x_- = x - t \quad (2.1)$$

When discretized, they define a light-cone lattice of “events” as in figure 2.1. Then, any rational and not

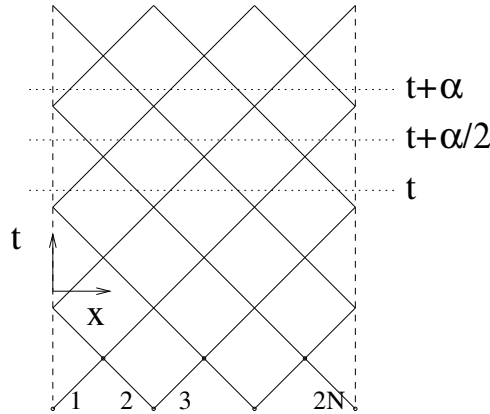


Figure 2.1. Light-cone lattice with periodic boundary conditions in space direction; states are associated to edges, enumerated from 1 to $2N$.

greater than 1 value is permitted as particle speed, in an infinite lattice. The shortest displacement of the particle (one lattice spacing) is realized at light speed ± 1 and corresponds, from the statistical point of view, to nearest neighbors interactions. Particles are therefore massless and can be right-movers (R) or left-movers (L) only. Smaller speeds can be obtained with displacements longer than the fundamental cell and correspond to higher neighbors interactions. They will not be used here. With only nearest neighbor interactions, the evolution from one row to the next one, as in figure 2.1, is governed by a

transfer matrix. Here there are four of them. Two act on the light-cone, U_R and U_L , the first one shifting the state of the system one step forward-right, the other one step forward-left. The remaining U and V^2 act in time and space directions respectively

$$U = e^{-i\alpha H} = U_R U_L, \quad V^2 = e^{-i\alpha P} = U_R U_L^\dagger \quad (2.2)$$

so they actually correspond to the Hamiltonian (forward shift) and the total momentum (right shift). Their action is pictorially suggested in figure 2.2. Also, the relations hold

$$U_R = e^{-i\frac{\alpha}{2}(H+P)}, \quad U_L = e^{-i\frac{\alpha}{2}(H-P)} \quad (2.3)$$

Much more details are given in [20] and on the original papers cited there. I now construct the alternating

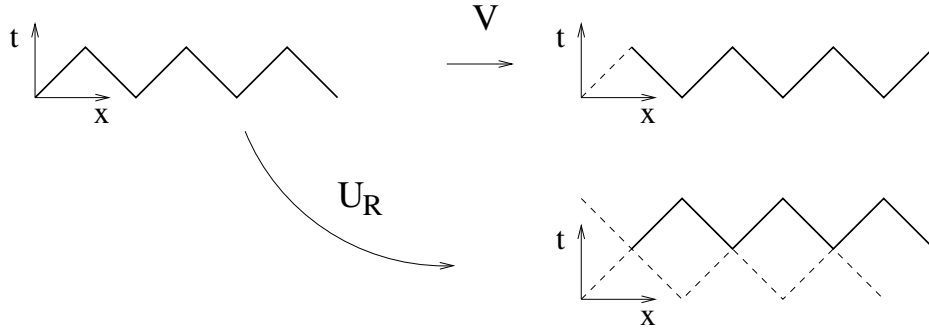


Figure 2.2. The action of the operators V and U_R is illustrated. The operator U_L acts as U_R but with leftward movement.

transfer matrix

$$\mathbf{T}(\theta, \Theta, \gamma_{6v}) = \text{Tr}_A L_1(\theta - \Theta) L_2(\theta + \Theta) \dots L_{2N-1}(\theta - \Theta) L_{2N}(\theta + \Theta) \quad (2.4)$$

where the operators L_i are associated to a vertex. To remove ambiguity, one has to associate odd numbers to the lower vertex, even numbers to the upper vertex, compare with Figure 2.1. Θ for the moment is a free parameter. Its presence corresponds to make the lattice model inhomogeneous such that the interaction on each site is tuned by the presence of the inhomogeneity. This does not change integrability. The standard construction of (1.30) suggest to take

$$L_i(\theta) = R_{Ai}(\theta) \quad (2.5)$$

using the R matrix of the six-vertex model (1.32). The forward-right and the forward-left operators are obtained by

$$U_R = \mathbf{T}(\Theta, \Theta, \gamma_{6v}), \quad U_L = \mathbf{T}(-\Theta, \Theta, \gamma_{6v}) \quad (2.6)$$

One can interpret these expressions by noticing that to switch from a right mover to a left mover one has to change the sign of rapidity. The transfer matrices depend on Θ and on the coupling γ_{6v} , whose values are not yet specified. The methods of Bethe ansatz can be used to diagonalize these operators as in the subsection 1.2.1. The specific case is treated in [21] and gives the following results. The eigenvalues of the transfer matrix are given by

$$\begin{aligned} T(\theta, \Theta) = & [a(\theta - \Theta) a(\theta + \Theta)]^N \prod_{j=1}^M \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} + \vartheta_j + \theta \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} - \vartheta_j - \theta \right]} + \\ & + [b(\theta - \Theta) b(\theta + \Theta)]^N \prod_{j=1}^M \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{3\pi}{2} - \vartheta_j - \theta \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[-i\frac{\pi}{2} + \vartheta_j + \theta \right]} \end{aligned} \quad (2.7)$$

provided the values of ϑ_j satisfy the set of coupled nonlinear equations called Bethe equations

$$\left(\frac{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j + \Theta + \frac{i\pi}{2} \right] \sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j - \Theta + \frac{i\pi}{2} \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j + \Theta - \frac{i\pi}{2} \right] \sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j - \Theta - \frac{i\pi}{2} \right]} \right)^N = - \prod_{k=1}^M \frac{\sinh \frac{\gamma_{6v}}{\pi} [\vartheta_j - \vartheta_k + i\pi]}{\sinh \frac{\gamma_{6v}}{\pi} [\vartheta_j - \vartheta_k - i\pi]} \quad (2.8)$$

where M can be any integer from 0 to N included. The complex numbers $\{\vartheta_j\}$ are called *Bethe roots*. These equations are a modification of (1.41). Because of the periodicity

$$\vartheta_j \rightarrow \vartheta_j + \frac{\pi^2}{\gamma_{6v}} i \quad (2.9)$$

further analyses can be restricted to a strip around the real axis

$$\vartheta_j \in \mathbb{R} \times i \left] -\frac{\pi^2}{2\gamma_{6v}}, \frac{\pi^2}{2\gamma_{6v}} \right]. \quad (2.10)$$

Details on Bethe equations and Bethe roots were given in subsection 1.2.1.

Another form of the Bethe equations can be obtained by taking the logarithm of the previous one. It is important to fix and consistently use a logarithm determination: here the fundamental one will be used. The equations become

$$\begin{aligned} 2\pi I_j &= N \log \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j + \Theta + \frac{i\pi}{2} \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j + \Theta - \frac{i\pi}{2} \right]} + N \log \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j - \Theta + \frac{i\pi}{2} \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[\vartheta_j - \Theta - \frac{i\pi}{2} \right]} \\ &- \sum_{k=1}^M \log \frac{\sinh \frac{\gamma_{6v}}{\pi} [\vartheta_j - \vartheta_k + i\pi]}{\sinh \frac{\gamma_{6v}}{\pi} [\vartheta_j - \vartheta_k - i\pi]} \end{aligned} \quad (2.11)$$

where their nature of quantization conditions is now explicit: the I_j are quantum numbers, taken half-integers or integers according to the parity of the number of Bethe roots

$$I_j \in \mathbb{Z} + \frac{1+M}{2} \quad (2.12)$$

The energy E and momentum P of a state can be read out from (2.3) and (2.7)

$$e^{i\frac{\alpha}{2}(E \pm P)} = \prod_{j=1}^M \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} - \Theta \pm \vartheta_j \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} + \Theta \mp \vartheta_j \right]} \quad (2.13)$$

or by the same equation in logarithmic form

$$E \pm P = -i\frac{2}{\alpha} \sum_{j=1}^M \log \frac{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} - \Theta \pm \vartheta_j \right]}{\sinh \frac{\gamma_{6v}}{\pi} \left[i\frac{\pi}{2} + \Theta \mp \vartheta_j \right]} \quad (2.14)$$

The logarithmic forms reveal an interesting aspect of the Bethe ansatz namely that energy, momentum, spin (see later) and all the higher integrals of motion have an additive structure in which Bethe roots resemble rapidities of independent particles

$$I_l = \sum_{j=1}^M f_l(\vartheta_j) \quad (2.15)$$

called “quasiparticles”. Quasiparticles are usually distinct from physical particles. They are degrees of freedom that do not appear in the Hamiltonian (1.35) but are “created” by the Bethe ansatz and incorporate the effects of the interactions. Indeed, their dispersion relation is not Galilean nor relativistic¹. Quasiparticles can have complex “rapidities”.

With this quasiparticle nature of Bethe roots in mind, the left hand side of the Bethe equations (2.8) is precisely the j th momentum term that one can extract from (2.14). The right hand side represents the interaction of pairs of quasi-particles.

In this Bethe ansatz description, the third component of the spin is given by

$$S_z = N - M \quad (2.16)$$

where the reference state for the algebraic Bethe ansatz is taken with all spins up or all spins down and it is described by $M = 0$ in (2.8): it is the ferromagnetic state. Then, every Bethe root corresponds to overturning a spin: it is a “magnon”, because it carries a unit of “magnetization”. It is also called spin wave. It is the smallest “excitation” of the ferromagnetic state. When $M = N$, all roots are real and one has the antiferromagnetic state, that is an ordered state with zero total spin but with a nontrivial local spin organization. Here, with the present sign conventions, it is also the ground state. Its actual expression is complicated. Just to give an idea of what it can look like, in the simplest case of an homogeneous ($\Theta = 0$) XXX ($\gamma_{6v} = 0$) model for a two-site chain it is

$$|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle \quad (2.17)$$

while for four sites it is

$$|\uparrow\uparrow\downarrow\downarrow\rangle + |\downarrow\downarrow\uparrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle + |\uparrow\downarrow\downarrow\uparrow\rangle - 2(|\uparrow\downarrow\downarrow\uparrow\rangle + |\downarrow\uparrow\uparrow\downarrow\rangle) \quad (2.18)$$

Excitations of the antiferromagnetic state are: (1) “real Bethe holes”, namely real positions corresponding to real roots in the antiferromagnetic state but excluded in the excitation, (2) complex roots.

In what follows, only the antiferromagnetic ground state and its excitations will be considered, because it has one important property: in the thermodynamic limit $N \rightarrow \infty$ it can be interpreted as a Dirac sea and the its excitations, holes and complex roots, behave as particles.

For later convenience, the coupling constant γ_{6v} is expressed in terms of a different variable p :

$$p = \frac{\pi}{\gamma_{6v}} - 1, \quad 0 < p < \infty \quad (2.19)$$

and I will work in the range of $0 < \gamma_{6v} < \pi$. Notice that, in (1.36) and in table 1.1, this is the choice that corresponds to the critical regime. In this new parameter, the strip becomes

$$\vartheta_j \in \mathbb{R} \times i \left] -\frac{\pi(1+p)}{2}, \frac{\pi(1+p)}{2} \right]. \quad (2.20)$$

This new parameter is related to the sine-Gordon ones by

$$p = \frac{\beta^2}{8\pi - \beta^2} \quad (2.21)$$

$0 < p < 1$ attractive regime; $1 < p < \infty$ repulsive regime

see also (1.16). With this parameter, the relation between the six-vertex and sine-Gordon coupling is

$$\gamma = 8\pi p = 8\pi \left(\frac{\pi}{\gamma_{6v}} - 1 \right) \quad (2.22)$$

Thus, the XXX chain is characterized by $\gamma_{6v} = 0$ that means $\beta^2 = 8\pi$. This is the strongest point in the repulsive regime of sine-Gordon. After that point, the quantum sine-Gordon model seems to loose meaning.

¹Galilean: $E = \frac{p^2}{2m}$, relativistic $E = \sqrt{p^2 c^2 + m^2 c^4}$.

2.2 A nonlinear integral equation from the Bethe ansatz

In this section the fundamental nonlinear integral equation driving sine-Gordon scaling functions will be presented. In the literature it is known with several names, following the different formulations that have been done: Klümper-Batchelor-Pearce equation or Destri-de Vega equation. It has also been indicated with the nonspecific tetragram NLIE (nonlinear integral equation). It was first obtained in [24] for the vacuum (antiferromagnetic ground state) scaling functions of XXZ then, with different methods, in [25] for XXZ and sine-Gordon. I will follow the Destri-de Vega approach applied to the sine-Gordon model.

The treatment of excited states was pioneered in [26] and refined in [27, 28], to arrive to the final form in [29, 20].

It is important to stress that this formalism is equivalent to the Bethe equations but is especially indicated to the antiferromagnetic regime. In general, it adapts to regimes where the number of Bethe roots is of the order of the size of the system. Indeed, the key idea is to sum up a macroscopically large number of Bethe roots for the ground state or for the reference state and replace them by a small number of holes to describe deviations near the reference state, as holes in a Dirac sea.

2.2.1 Counting function

First, it is possible to write the Bethe equations (2.11) in terms of a *counting function* $Z_N(\vartheta)$. I introduce the function

$$\phi_\nu(\vartheta) = i \log \frac{\sinh \frac{1}{p+1}(i\pi\nu + \vartheta)}{\sinh \frac{1}{p+1}(i\pi\nu - \vartheta)}, \quad \phi_\nu(-\vartheta) = -\phi_\nu(\vartheta)$$

The “oddity” on the analyticity strip around the real axis defines a precise logarithmic determination. The counting function is defined by

$$Z_N(\vartheta) = N[\phi_{1/2}(\vartheta + \Theta) + \phi_{1/2}(\vartheta - \Theta)] - \sum_{k=1}^M \phi_1(\vartheta - \vartheta_k) \quad (2.23)$$

The logarithmic form of the Bethe equations (2.11) takes now a simple form in terms of the counting function

$$Z_N(\vartheta_j) = 2\pi I_j, \quad I_j \in \mathbb{Z} + \frac{1+\delta}{2}, \quad \delta = (M) \bmod 2 = (N - S_z) \bmod 2 \in \{0, 1\} \quad (2.24)$$

Notice that the counting function is not independent of the Bethe roots. Said differently, one cannot separate the construction of Z_N and the solution of (2.24). Now it is possible to give a formal definition of “holes”: they are solutions of (2.24) that do not appear in (2.23). I will not make use of nonreal holes. Bethe roots and holes are zeros of the equation

$$1 + (-1)^\delta e^{iZ_N(\vartheta_j)} = 0 \quad (2.25)$$

once the counting function is known. More, they are simple zeros because Bethe roots/holes exclude each other.

2.2.2 Classification of Bethe roots and counting equation

From Bethe Ansatz it is known that a solution of (2.11), namely a Bethe state, is uniquely characterized by the set of quantum numbers $\{I_j\}_{j=1,\dots,M}$, $0 \leq M \leq N$ that appear in (2.24). Notice that $M \leq N$ means $S \geq 0$.

Bethe roots can either be real or appear in complex conjugate pairs. Complex conjugate pairs grant the reality of the energy, momentum and transfer matrix. In the specific case (2.8), there is another possibility, due to the periodicity (2.9): if a complex solution has imaginary part $\text{Im } \vartheta = \frac{\pi}{2}(p+1)$, it

can appear alone (its complex conjugate is not required). A root with this value of the imaginary part is called *self-conjugate root*.

From the point of view of the counting function, a more precise classification of roots is required:

- *real roots*; they are real solutions of (2.24); their number is M_R ;
- *holes*; real solutions of (2.24) that do appear in the ground state but not in the excitation under examination; in practice, they are real of (2.24) that do not enter in the counting function (2.23); their number is N_H ;
- *special roots or holes* (special objects); they are real roots or holes whose counting function derivative $Z'_N(\vartheta_j)$ is negative, contrasted with normal roots or holes, whose derivative is positive; their number is N_S ; they must be counted both as “normal” and as “special” objects;
- *close pairs*; complex conjugate solutions with imaginary part in the range $0 < |\text{Im } \vartheta| < \pi \min(1, p)$; this range is dictated by the first singularity (essential singularity) of the function $\phi_1(\theta)$, when moving of the real axis; their number is M_C ;
- *wide roots in pairs*: complex conjugate solutions with imaginary part belonging to the range $\pi \min(1, p) < |\text{Im } \vartheta| < \pi \frac{p+1}{2}$ namely after the first singularity of $\phi_1(\theta)$;
- *self-conjugate roots*: complex roots with imaginary part $\text{Im } \vartheta = \pi \frac{p+1}{2}$; they are wide roots but miss the complex conjugate so they are single; their number is M_{SC} .

The total number of wide roots appearing in pairs or as single is M_W . The following notation will be used, sometimes, for later convenience, to indicate the position of the solutions: h_j for holes, y_j for special objects, c_j for close roots, w_j for wide roots.

Complex roots with imaginary part larger than the self-conjugates are not required because of the periodicity of Bethe equations (2.10). A graphical representation of the various types of solutions is given in figure 2.3.

The function Z_N (2.23) has a number of branch point singularities produced by the presence of the logarithms. The largest horizontal strip containing the real axis and free of singularities is bounded by the singularities of the various terms $\phi_\nu(\vartheta)$. The strip is at the largest size when no complex roots are introduced, otherwise it is narrower because the imaginary part of the complex roots in $\phi_\nu(\vartheta - \vartheta_k)$ displaces the position of the singularities.

An important property follows from this classification: the Z_N function is *real analytic* in a strip that contains the real axis

$$Z_N(\vartheta^*) = (Z_N(\vartheta))^* \quad (2.26)$$

By considering asymptotic values of $\phi_\nu(\vartheta)$ and $Z_N(\vartheta)$ for $\vartheta \rightarrow \pm\infty$, it is possible to obtain an equation relating the numbers of all the various types of roots. I refer the reader interested in the details of the derivation to [27, 20]. Here I only mention the final result, in the form where the continuum limit $N \rightarrow \infty$, $a \rightarrow 0$ and $L = Na$ finite, has already been taken

$$N_H - 2N_S = 2S_z + M_C + 2\theta(p-1)M_W \quad (2.27)$$

where $\theta(x)$ is the step function: $\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$. Recall that S_z is a nonnegative integer and the right hand side only contains nonnegative values. From this, it turns out that N_H is even (M_C is the number of close roots, and is even). This *counting equation* expresses the fact that the Bethe equations have a finite number of solutions only. There are also other constraints, once N is fixed:

$$S_z \leq N, \quad M_C + M_W \leq N, \quad N_H \leq N. \quad (2.28)$$

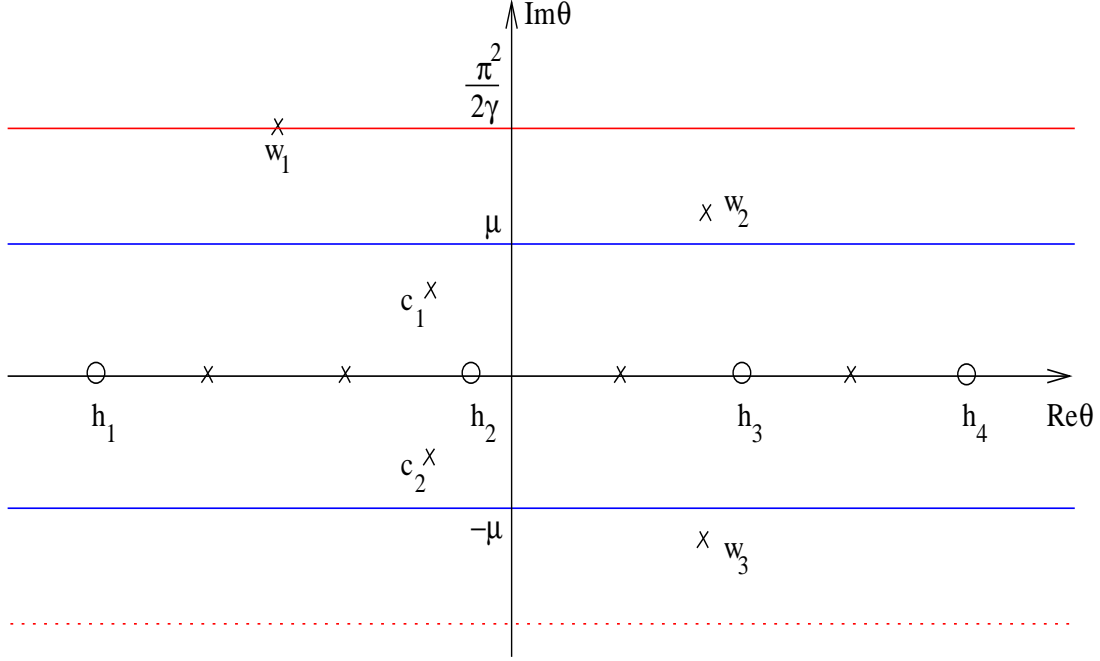


Figure 2.3. The different types of roots and holes and their position in the complex plane. We denote $\mu = \pi \min(1, p)$. The red line at $\frac{\pi^2}{2\gamma^{6v}} = \frac{\pi}{2}(p+1)$ is the self-conjugate one. Close roots are located within the blue lines, wide roots lie outside. The holes are indicated by the circles on the real axis.

Moreover, the various types of roots/holes do respect the mutual exclusion principle. This means that, in order to accommodate complex roots, one has to “create” space by inserting holes, or vice versa.

Notice also that in the attractive regime the wide roots do not participate to the counting and that at the free fermion point $p = 1$, or $\beta^2 = 4\pi$, they do exist as self-conjugate only, namely there are no wide roots in pairs. This suggests that the role of wide roots is different in the two regimes.

The most important fact is that the number of real roots does not appear in this equation: they have been replaced by the number of holes. This, together to what will be explained in the next paragraph, allows to consider the real roots as a sea of particles, or Dirac sea, and all other types of solutions, holes and complex roots, as excitations above it.

2.2.3 Nonlinear integral equation

Let \hat{x} be a real solution of the Bethe equation. Thanks to Cauchy’s integral formula, an holomorphic function $f(x)$ admits the following representation

$$f(\hat{x}) = \oint_{\Gamma_{\hat{x}}} \frac{d\mu}{2\pi i} \frac{f(\mu)}{\mu - \hat{x}} = \oint_{\Gamma_{\hat{x}}} \frac{d\mu}{2\pi i} f(\mu) \frac{(-1)^\delta e^{iZ_N(\mu)} iZ'_N(\mu)}{1 + (-1)^\delta e^{iZ_N(\mu)}} \quad (2.29)$$

where $\Gamma_{\hat{x}}$ is an anti-clockwise simple path encircling \hat{x} , namely one of the real holes or complex roots, and avoiding all the others, see (2.25). In the region where $\phi_1(\vartheta)$ is holomorphic, (2.29) can be used to write an expression for all the real roots and real holes

$$\begin{aligned} \sum_{k=1}^{M_R+N_H} \phi_1(\vartheta - x_k) &= \sum_{k=1}^{M_R+N_H} \oint_{\Gamma_{x_k}} \frac{d\mu}{2\pi i} \phi_1(\vartheta - \mu) \frac{(-1)^\delta e^{iZ_N(\mu)} iZ'_N(\mu)}{1 + (-1)^\delta e^{iZ_N(\mu)}} = \\ &= \oint_{\Gamma} \frac{d\mu}{2\pi i} \phi_1(\vartheta - \mu) \frac{(-1)^\delta e^{iZ_N(\mu)} iZ'_N(\mu)}{1 + (-1)^\delta e^{iZ_N(\mu)}} \end{aligned} \quad (2.30)$$

The sum on the contours has been modified to a unique curve Γ encircling all the real solutions x_k (real root plus holes), and avoiding the complex Bethe solutions as in the Figure 2.4; this is possible because they are finite in number.

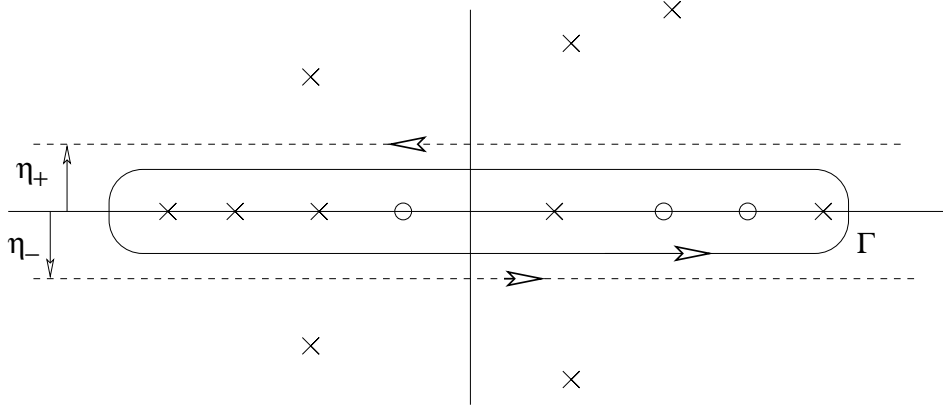


Figure 2.4. The integration curve encircles real solutions only. The crosses represent roots while the circles represent holes.

Clearly the Γ curve must be contained in the strip

$$0 < \eta_+, \eta_- < \min\{\pi, \pi p, |\text{Im } c_k| \forall k\}$$

Without loss of generality, assume that $\eta_+ = \eta_- = \eta$, and deform Γ to the contour of the strip characterized by η . The regions at $\pm\infty$ do not contribute because, as the lattice size is finite, those regions are free of root or holes. Moreover, in those regions, Z'_N vanishes therefore the integral can be just evaluated on the lines $\mu = x \pm i\eta$, where x is real. After algebraic manipulations involving integrations by parts and convolutions (for details see [20]) one arrives at a nonlinear integral equation for the counting function $Z_N(\vartheta)$

$$\begin{aligned} Z_N(\vartheta) = & 2N \arctan \frac{\sinh \vartheta}{\cosh \Theta} + \sum_{k=1}^{N_H} \chi(\vartheta - h_k) - 2 \sum_{k=1}^{N_S} \chi(\vartheta - y_k) - \\ & - \sum_{k=1}^{M_C} \chi(\vartheta - c_k) - \sum_{k=1}^{M_W} \chi(\vartheta - w_k)_{II} + \\ & + 2 \text{Im} \int_{-\infty}^{\infty} d\rho G(\vartheta - \rho - i\eta) \log \left(1 + (-1)^\delta e^{iZ_N(\rho + i\eta)} \right) \end{aligned} \quad (2.31)$$

The kernel

$$G(\vartheta) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk e^{ik\vartheta} \frac{\sinh \frac{\pi(p-1)k}{2}}{2 \sinh \frac{\pi p k}{2} \cosh \frac{\pi k}{2}} \quad (2.32)$$

presents a singularity at the same place where $\phi_1(\vartheta)$ does: $\vartheta = i\pi \min\{1, p\}$. An analytic continuation outside the fundamental strip $0 < |\text{Im } \vartheta| < \pi \min\{1, p\}$ (I determination region) must take this fact into account. The source terms are given by

$$\chi(\vartheta) = 2\pi \int_0^\vartheta dx G(x)$$

and

$$\chi(\vartheta)_{II} = \begin{cases} \chi(\vartheta) + \chi(\vartheta - i\pi \text{sign}(\text{Im } \vartheta)) , & p > 1 , \\ \chi(\vartheta) - \chi(\vartheta - i p \pi \text{sign}(\text{Im } \vartheta)) , & p < 1 . \end{cases} \quad (2.33)$$

is a modification of the source term due to the analytic continuation over the strip $0 < |\text{Im } \vartheta| < \pi \min\{1, p\}$, i.e. in the so called II determination region.

Such equation, together with the quantization condition (2.24), is equivalent to the original Bethe Ansatz (2.8). The NLIE for Z_N is not independent of the Bethe roots: it and the quantization conditions must be solved at the same time. Once the Bethe roots are known, one can use them into eqs.(2.13) to compute the energy and momentum of a given state.

2.2.4 Continuum limit

Although such NLIE is already a precious tool for the lattice model itself, its importance becomes essential when a continuum limit is done.

The continuum limit has the objective to transform a lattice system into a continuum model. As already mentioned, one has to take the lattice size $N \rightarrow \infty$ (that would be the normal thermodynamic limit of statistical mechanics) and the lattice edge $\alpha \rightarrow 0$ simultaneously, in such a way that the product $L = N\alpha$ stays finite. In this way one obtain a continuum theory with finite size space, namely a cylindrical geometry. However, the lattice spacing is not present in the Boltzmann weights and in the transfer matrix (2.4, 1.32) so we have no way to use it. Moreover, one can convince himself, by explicit calculations, that if the limit is taken by keeping the Θ parameter fixed, the lattice NLIE blows up to infinity and loses meaning. This reflects the fact that the number of roots increases as N in the thermodynamic limit. However, as shown in ref.[19], if one assumes a dependence of Θ on N of the form

$$\Theta \approx \log \frac{4N}{\mathcal{M}L}. \quad (2.34)$$

it is possible to get a finite limit out of the lattice NLIE. This limit is exactly the one that was used in [19] to bring a lattice fermion field into the Thirring fermion field on the continuum. Notice that sending $\Theta \rightarrow \infty$ in this way naturally introduces a renormalized physical mass \mathcal{M} . This is the deep reason of the use of the light-cone lattice and of the inhomogeneity in (2.4). In other words, without the inhomogeneity, the continuum system would be a critical one, massless, with central charge $c = 1$ ([24]).

The *continuum counting function* is defined by:

$$Z(\vartheta) = \lim_{N \rightarrow \infty} Z_N(\vartheta) \quad (2.35)$$

and appears in a continuum NLIE

$$Z(\vartheta) = l \sinh \vartheta + g(\vartheta|\vartheta_j) + 2\text{Im} \int_{-\infty}^{\infty} dx G(\vartheta - x - i\eta) \log \left(1 + (-1)^\delta e^{iZ(x+i\eta)} \right) \quad (2.36)$$

where $l = \mathcal{M}L$. The first term on the right hand side is a momentum term. The second one, $g(\vartheta|\vartheta_j)$, is a source term, in the sense that it adapts to the different combinations of roots and holes

$$g(\vartheta|\vartheta_j) = \sum_{k=1}^{N_H} \chi(\vartheta - h_k) - 2 \sum_{k=1}^{N_S} \chi(\vartheta - y_k) - \sum_{k=1}^{M_C} \chi(\vartheta - c_k) - \sum_{k=1}^{M_W} \chi(\vartheta - w_k)_{II} \quad (2.37)$$

The positions of the sources $\{\vartheta_j\} \equiv \{h_j, y_j, c_j, w_j\}$ are fixed by the Bethe quantization conditions

$$Z(\vartheta_j) = 2\pi I_j \quad , \quad I_j = \mathbb{Z} + \frac{1+\delta}{2} \quad (2.38)$$

The parameter δ can be both 0 or 1. On the lattice it was determined by the total number of roots, which now has become infinite. Restrictions on it will appear later. The vacuum state, or Hamiltonian ground state, corresponds to the choice $\delta = 0$.

With a procedure analogous to the one sketched above, it is possible to produce integral expressions for energy and momentum. Starting from (2.13), one has to isolate an extensive term, proportional to N , to be subtracted. The remaining finite part of energy and momentum takes the form

$$E - E_{bulk} = \mathcal{M} \left(\sum_{j=1}^{N_H} \cosh h_j - 2 \sum_{j=1}^{N_S} \cosh y_j - \sum_{j=1}^{M_C} \cosh c_j + \sum_{j=1}^{M_W} (\cosh w_j)_{II} - \int_{-\infty}^{\infty} \frac{dx}{2\pi} 2 \operatorname{Im} \left[\sinh(x + i\eta) \log(1 + (-1)^\delta e^{iZ(x+i\eta)}) \right] \right) \quad (2.39)$$

$$P = \mathcal{M} \left(\sum_{j=1}^{N_H} \sinh h_j - 2 \sum_{j=1}^{N_S} \sinh y_j - \sum_{j=1}^{M_C} \sinh c_j + \sum_{j=1}^{M_W} (\sinh w_j)_{II} - \int_{-\infty}^{\infty} \frac{dx}{2\pi} 2 \operatorname{Im} \left[\cosh(x + i\eta) \log(1 + (-1)^\delta e^{iZ(x+i\eta)}) \right] \right) \quad (2.40)$$

Therefore, energy and momentum can be evaluated once the counting function $Z(\vartheta)$ and the source positions ϑ_j have been obtained from (2.36, 2.38). All these equations are exact, no approximation has been introduced in deriving them.

In practice, these equations can be treated analytically in certain limits ($l \rightarrow 0$ or $l \rightarrow \infty$) and numerically for intermediate values, where we actually lack a closed formula for them. Numerical computations are done without any approximation other than the technical ones introduced by the computer truncations. In calculations, one starts from an initial guess for the counting function, $Z^{(0)}(\vartheta)$, uses it in (2.38) to get the roots/holes positions then evaluates a new $Z^{(1)}(\vartheta)$ from (2.36) and so on, up to the required precision. This iterative procedure is conceptually very simple and inclined to good convergence, as one can easily estimate. Indeed, the following term appears within integration

$$e^{iZ(x+i\eta)} \approx e^{iZ - \eta l \cosh x} \quad (2.41)$$

The presence of a negative cosh at the exponent makes the support of the integral compact and the integral itself subdominant with respect to all the other terms, speeding up the convergence of the iteration, especially for large l .

So, at least for the cases where holes only are considered, and no complex roots or no special roots, finding numerical solutions can be quite easy. The whole procedure takes few seconds of computing on a typical Linux/Intel platform without resorting to any supercomputer or other technically advanced tool.

When complex roots are present, things are much more complicated and the computation time increases dramatically. Also, convergence at small l can be problematic because those real roots or holes that are closer to the origin can become “special”. In practice, they emanate one or two “supplementary” sources in consequence of a local change of sign of $Z'(x)$. They have not been extensively treated. A similar phenomenon has been discussed in [56], in the frame of thermodynamic Bethe ansatz.

The limit procedure described here is mathematically consistent, but the question is if from the physical point of view it describes a consistent quantum theory and allows for a meaningful physical interpretation.

The first indication comes from the emergence, in [19], of the fermionic massive Thirring fields from the six-vertex diagonal alternating lattice of section 2.1. This indicates that the procedure points toward a sine-Gordon/massive Thirring model.

Before going on, an important remark must be made about the allowed values for the XXZ spin S_z . From (2.16), only nonnegative integer values can be given to S_z .

As shown in [30], one is led to include also the half-integer choice for S_z , in order to describe the totality of the spectrum. This choice seems not justified on the light-cone lattice of section 2.1 because it would require adding one column of points to the lattice, thus spoiling periodicity. Most probably the way to introduce it would be by inserting a twist in the seam or some other nontrivial boundary condition.

In any case, half-integer values for S_z are necessary and seem fully consistent with the rest of the model to describe odd numbers of particles.

At this point the following physical scenario appears.

1. The physical vacuum, or ground state, of the continuum theory comes from the antiferromagnetic state of the lattice so is characterized by the absence of sources, holes or complex roots.
2. All the sources are excitations above this vacuum.
3. This theory describes at least the sine-Gordon and the massive Thirring model on a cylinder; the circumference describes a finite space of size L ; the infinite direction is time S_z is the topological charge and can take nonnegative integer or half-integer values.
4. This theory describes also states that are not in sine-Gordon or in massive Thirring.

As already observed, the real roots have disappeared from the counting equation in the continuum limit. They actually become a countable set and are taken into account by the integral term, both in the NLIE and in the energy-momentum expressions. They can be interpreted as a sort of Dirac sea on which holes and complex roots build particle excitations. Of course, the presence of holes or complex roots distorts the Dirac sea too, through the source term $g(\vartheta|\vartheta_j)$.

Observe that it has been indicated that only nonnegative values of S_z are required to describe the whole Hilbert space of the theory. Indeed the lattice theory is assumed charge-conjugation invariant so negative values of S_z , namely states with negative topological charge, have the same energy and momentum as their charge conjugate states.

The assumption that all the sine-Gordon and all massive Thirring states can be described by the NLIE is absolutely not trivial and still misses a mathematical proof even if all the analyses done so far are consistent with this assumption.

2.2.5 The infrared limit of the NLIE and the particle scattering

The first task in order to understand the physics underlying the NLIE is to characterize the scattering of the model, by reconstructing the S-matrix. As we started from an integrable model, we assume that the continuum one remains integrable. We will find that this hypothesis is extremely reasonable because it is related to the structure of the source term $g(\theta|\theta_i)$. Indeed, the function χ can be written as

$$\chi(\vartheta) = -i \log S(\vartheta) \quad (2.42)$$

where $S(\vartheta)$ is the soliton-soliton scattering amplitude in sine-Gordon theory 1.27, if the parameters are fixed as in (2.19). This means that the exponentiation of the source (2.37) term is the product of several sine-Gordon two-particle scattering amplitudes, as it appears in the factorization theorem.

One has to remember that the theory has been constructed on a cylinder therefore the connection with the factorization theorem can emerge only in the limit where the circumference becomes infinite. In this limit, the cylinder becomes indistinguishable from a plane. Here the only external parameter is the adimensional “size” $l = \mathcal{M}L$. It will be pushed to infinity $l \rightarrow \infty$. This can be interpreted as a very large volume or a very large mass, thus explaining the name of infrared limit (IR).

In this limit, the integral terms in (2.36) and in (2.39, 2.40) vanish exponentially fast, so they can be dropped and one remains with the momentum and the source term. Indeed, one can estimate that

$$\log(1 + (-1)^\delta e^{iZ(x+i\eta)}) \approx \log(1 + (-1)^\delta e^{iZ - \eta l \cosh x}) \approx (-1)^\delta e^{iZ - \eta l \cosh x} \quad (2.43)$$

The presence of a negative cosh at the exponent produces an exponentially fast decay for large l in the integral terms.

Consider first a state with N_H holes only and XXZ spin $S_z = N_H/2$.

$$Z(\vartheta) = l \sinh \vartheta + \sum_{j=1}^{N_H} \chi(\vartheta - h_j) \quad , \quad Z(h_j) = 2\pi I_j \quad (2.44)$$

This equation is the quantization of momenta in a box, for a system of particles. Indeed, by exponentiation one has

$$\exp(i l \sinh h_k) \prod_{j=1}^{N_H} S(h_k - h_j) = \pm 1 \quad (2.45)$$

where the sign depends on the parity of the quantum numbers. This leads to interpret holes as solitons with rapidities h_j . This is further evidenced by considering the energy and momentum expressions

$$E = \mathcal{M} \sum_{j=1}^{N_H} \cosh h_j \quad P = \mathcal{M} \sum_{j=1}^{N_H} \sinh h_j \quad (2.46)$$

which is the energy of N_H free particles of mass \mathcal{M} . The identification with the particular element $S(\theta)$ of the S-matrix forces to give to these solitons a topological charge $Q = +1$ each, which is consistent with the interpretation that $Q = 2S_z$. An analogous interpretation is possible in terms of pure antisolitons, reflecting the charge conjugation invariance of the theory.

When considering two holes and a complex pair, the source terms can be arranged, thanks to some identities satisfied by the functions χ , in the form

$$Z(\vartheta_i) = l \sinh(\vartheta_i) - i \log S_+(\vartheta_i - \vartheta_j) = 2\pi I_j \quad , \quad i, j = 1, 2$$

where

$$S_+(\vartheta) = \frac{\sinh\left(\frac{\vartheta+i\pi}{2p}\right)}{\sinh\left(\frac{\vartheta-i\pi}{2p}\right)} S(\vartheta)$$

which is the scattering amplitude of a soliton on an antisoliton in the parity-even channel. The quantum numbers I_+, I_- of the two complex roots are constrained to be $I_{\pm} = \mp \frac{1}{2}$ for consistency of the IR limit. This state has $S_z = 0$, with topological charge $Q = 0$.

There is an analogous parity-odd channel in sine-Gordon [2], with an S_- amplitude. It is realized by the state with two holes and a selfconjugate root. In the same way, it has been possible to treat more complex cases, with different combinations of roots [32]. See also [31] for details of the calculation. In the attractive regime one has also to consider the breather particles that appear as soliton-antisoliton bound states. It turns out that the breathers are represented by self-conjugate roots (1st breather) or by arrays of wide roots (higher breathers).

Thus, the whole scattering theory of sine-Gordon can be reconstructed in the IR limit, thanks to the structure of the source term. It is now difficult to argue that the NLIE does not describe sine-Gordon.

2.2.6 UV limit and vertex operators

It is interesting to study the opposite limit $l \rightarrow 0$, where one expects to see a conformal field theory; indeed, in this limit the masses vanish and scale invariance appears. This reproduces the UV limit of sine-Gordon/massive Thirring, namely the $c = 1$ conformal field theory described in section 1.3 and in the Figure 1.2.

The UV calculations are usually more difficult to perform than the IR ones, as they require to split the NLIE into two independent “left” and “right” parts, called *kink equations*. They correspond to the left and right movers of a two-dimensional conformal field theory. A similar manipulation is done on the energy and momentum expressions, that can finally be expressed in a closed form, thanks to a lemma

presented in [25]. For the details, the reader is invited to consult the thesis [20] where all the calculations are shown in detail. In the present text, I give only the main results and the physical insight they imply.

A first important result is that the $c = 1$ CFT quantum number m of the vertex operators (1.51), which is identified with the UV limit of the topological charge, can be related unambiguously to the XXZ spin by $\pm m = 2S_z$. Of course, the \pm reflects the charge conjugation invariance of the theory. Then, by examining the states already “visited” at the IR limit, one can establish a bridge between particle states and vertex operators of $c = 1$ theory.

1. The **vacuum** state has no sources, namely no holes or complex roots: only the sea of real roots is present. There are two possible choices: $\delta = 0$ or 1 . The result of the UV calculation gives

$$\begin{aligned} \text{for } \delta = 0 : \quad \Delta^\pm &= 0 & \text{i.e. } \mathbb{I} \\ \text{for } \delta = 1 : \quad \Delta^\pm &= \frac{1}{8R^2} & \text{i.e. } V_{(\pm 1/2, 0)} \end{aligned}$$

i.e. the physical vacuum is the one with $\delta = 0$. The other state belongs to the sector IV that does not describes a local CFT, as in Figure 1.2.

2. The **two-soliton** state, described by two holes, with the smallest quantum numbers, gives

$$(a) \text{ for } \delta = 0 \text{ and } I_1 = -I_2 = \frac{1}{2} \implies \Delta^\pm = \frac{R^2}{2} \text{ i.e. } V_{(0,2)}.$$

$$(b) \text{ for } \delta = 1 \text{ and } I_1 = -I_2 = 1 \implies \text{a } V_{(\pm 1/2, 2)} \text{ descendent, not in UV sG spectrum, as it also belongs to sector IV.}$$

3. The **symmetric soliton-antisoliton** state (two holes and a self-conjugate root), $\delta = 1$, $I_1 = -I_2 = 1$ and $I_c^\pm = 0 \implies \Delta^\pm = \frac{1}{2R^2}$ i.e. $V_{(\pm 1, 0)}$

4. The **antisymmetric soliton-antisoliton** state (two holes and a complex pair)

$$\delta = 0, I_1 = I_c^- = -I_2 = -I_c^+ = \frac{1}{2} \implies \Delta^\pm = \frac{1}{2R^2} \text{ i.e. } V_{(\pm 1, 0)}$$

It is obvious that these last two give two linearly independent combinations of the operators $V_{(\pm 1, 0)}$, one with even, the other with odd parity.

5. The **one hole** state with $I = 0$, $\delta = 1 \implies \Delta^\pm = \frac{1}{8R^2}$ i.e. the vertex operator $V_{(0,1)}$, belongs to sector II. For $\delta = 0$ there are two minimal rapidity states with $I = \pm \frac{1}{2}$. They are identified with the operators $V_{(\pm 1/2, \pm 1)}$. As these states belong to sector III, they are of fermionic nature and actually one identifies them with the components of the Thirring fermion.

These examples, taken all together, suggest the following choice of δ to discriminate between sine-Gordon and massive Thirring states

$$\begin{aligned} 2S_z + \delta + M_{SC} &\in 2\mathbb{Z} & \text{for Sine-Gordon} \\ \delta + M_{SC} &\in 2\mathbb{Z} & \text{for massive Thirring} \end{aligned} \quad (2.47)$$

where M_{SC} is the number of selfconjugate roots. This selects the sectors I and II for sine-Gordon states, and the sectors I and III for the Thirring ones, as in section 1.3. The NLIE describes also the sector IV, that does not contain local operators. The correct interpretation of Coleman equivalence of Sine-Gordon and Thirring models is that even topological charge sectors are identical, the difference of the two models shows up only in the odd topological charge sectors, for which the content of Thirring must be fermionic while that of Sine-Gordon must be bosonic.

To conclude these remarks, I briefly add a comment about the special objects that were introduced in the classification of roots but not really used later. I need to recall their definition: they are real roots or holes y_i having $Z'(y_i) < 0$. Now, the function Z is globally monotonically increasing. Indeed its asymptotic values for $\vartheta \rightarrow \pm\infty$ are dominated by the term $l \sinh \vartheta$ which is obviously monotonically increasing. Also, for l large, this term dominates. Therefore at IR the function Z is surely monotonic

and no special objects can appear. However, these global asymptotic estimations can fail at small l and finite ϑ . In that case the derivative $Z'(x)$ can become locally negative. Thus, a real root or hole with negative derivative becomes “special” (and splits in three objects). At the critical value l_{crit} of the parameter l , at which the derivative become negative moving from IR towards UV, the convergence of the iterative procedure breaks down, thus revealing that some singularity has been encountered. For the scaling function to be consistently continued after this singularity, one needs to modify the NLIE adding exactly the contributions that have been called special objects. A more careful analysis [20] reveals that these singularities are produced by the logarithm in the convolution term going off its fundamental determination: “special” objects are an artifact of the description by a counting function, they do not exist in the Bethe equations. A treatment of these objects can be found in [20]. See also the discussion at page 34. I don’t know of successful numerical calculations in presence of special objects. In [56] a similar case occurred in the TBA formalism, in presence of boundary interactions, and was treated numerically because it was localised in some asymptotic region.

2.3 Discussion

In this chapter I have introduced the formalism of Destri-de Vega to study the sine-Gordon model on a cylinder with finite size space and infinite time. The presentation proposed here has mainly the purpose to show that this method is effective in treating finite size effects in quantum field theory and creating a bridge from a massive field theory on Minkowski space-time (visible in the IR limit) to a conformal field theory.

As typical in treating integrable models, different systems meet on the way: lattice systems, scattering theory and conformal field theory all participate to the scenario described by the NLIE.

The formalism was introduced by Klümper et al. in [24] and by Destri and de Vega in [25]. After, a number of other people participated to its development. Particularly, my involvement characterized my PhD years from 1996 to 1999, with the Bologna group.

I directly contributed to four papers, [28], [29], [30], [32] and I wrote my PhD thesis on this subject [20]. The main steps of my contribution are

- The whole formulation was revisited and corrected.
- The study of the IR and UV limits was done systematically.
- The spectrum of the continuum theory was carefully described, using both UV, IR and numerical calculations. also adding the odd particle sector.
- Many cases were studied numerically, to gain a complete control of the whole region that separates the IR and the UV.
- The results were compared with perturbative calculations done with the truncated conformal space approach, giving a confirmation of the methods.
- The introduction of a twist allowed to describe the restrictions of sine-Gordon, namely the perturbation of conformal minimal models by the thermal operator. These are massive theories that are described by the same sine-Gordon NLIE after the introduction of an appropriate twist.

Later, other groups profited of this NLIE to investigate a variety of models. An unexpected development will be presented in chapter 4 and investigates integrability-related problems in gauge theory (especially $\mathcal{N} = 4$ SYM).

Are there other things to be done? Even if the degree of difficulty is very high, the gain would be great, if one could succeed in the description of the eigenvectors in the continuum theory, or of some correlation function. Their knowledge is important because they enter into the evaluation of many

physical quantities (diffusion amplitudes, magnetic susceptibility) whose values can be compared with experiments.

Chapter 3

Thermodynamic Bethe Ansatz

The first treatment of Bethe equations in their thermodynamic limit was done by Yang and Yang in [34], for a system of nonrelativistic bosons interacting by a repulsive delta-function, on a line. The Bethe equations were obtained from the model Hamiltonian by the coordinate Bethe ansatz calculation, one of the several implementations of the Bethe ansatz methods. Then, the objective of that treatment was to evaluate the thermodynamic limit of the Bethe equations. The authors succeeded and were able to get the partition function of this interacting gas. They also showed the partition function analyticity in the temperature and the chemical potential, indicating the absence of phase transitions.

This method was generalized by A.I.B. Zamolodchikov [35] for relativistic particles interacting with a factorized scattering matrix. His goal was to create a contact between a factorized scattering theory of a given S matrix to its ultraviolet limit, typically a conformal field theory in two dimensions. The author reasonably assumes that, at a finite temperature, the equilibrium states of the particles in a box are described by some Bethe-like wave functions (asymptotic wave function), precisely as in the Yang and Yang approach. A quantization condition inspired to Bethe equations (1.41, 2.8) is thus imposed. Indeed, in the Bethe equations structure we have recognized a momentum term and an interaction term, see near (2.15). Zamolodchikov assumes that the interaction term is given by a factor of S matrix amplitudes and the momentum is the usual relativistic one. Notice, however, that the true Bethe wave functions obtained within Bethe ansatz calculations involve “quasiparticles”, as described near (2.15), while the scattering theory involves physical particles. For example, the Bethe roots can be complex while physical particle rapidities are always real. The assumption works and the Zamolodchikov “thermodynamic Bethe ansatz” has been applied to a variety of models. It allows to study the theory obtained by perturbing a conformal field theory with a relevant operator, under the condition that the perturbation maintains integrability.

Later, Pearce and Klümper in [36] introduced another approach to “calculate analytically the finite-size corrections and scaling dimensions of critical lattice models” (quoted from [36]). These authors do not make use of Bethe equations; instead, they start from the transfer matrix of an integrable lattice model and, knowing the arrangement of the zeros of its eigenvalues, are able to solve certain identities satisfied by the transfer matrix itself. Then, one can evaluate the continuum limit of lattice models.

In the following, I will mainly talk about the last approach. All of them have triggered several further investigations. Indeed, the TBA serves as an interface between conformally invariant theories and massive or massless integrable theories, in particular when these massive or massless theories are obtained as deformations of the conformal ones.

3.1 Lattice TBA

I start by defining a family of models on a square lattice of N horizontal cells (faces) and with many rows (their number will not be used) using the following diagrammatic representation for the double row

transfer matrix [37]

$$D(N, u, \xi)_{\sigma \sigma'} = \sum_{\tau_0, \dots, \tau_{N-1}} \begin{array}{c} \begin{array}{c} r \\ \lambda - u \\ \xi \\ r \end{array} \begin{array}{|c|c|c|c|c|c|} \hline \sigma'_1 & \sigma'_2 & \sigma'_3 & & \sigma'_{N-1} & 1 \\ \hline \lambda - u & \lambda - u & \lambda - u & & & \lambda - u \\ \hline \tau_0 & \tau_1 & \tau_2 & \tau_3 & \tau_{N-1} & \tau_N \\ \hline u & u & u & & & u \\ \hline \sigma_1 & \sigma_2 & \sigma_3 & & \sigma_{N-1} & 1 \end{array} \end{array} \quad (3.1)$$

I use a double row transfer matrix [42] because, in presence of boundary interactions, it is needed to ensure integrability. In fact, it is a transfer matrix that acts from the row i to the $i + 2$ while in a more standard single row transfer matrix it would act from i to $i + 1$.

The diagrammatic representation is a mean to simplify the notation and to reduce the use of indices; it is also quite effective to realize a sort of “graphical algebra”, useful to verify a number of properties [37]. An entry of the transfer matrix, $D(N, u, \xi_{\text{latt}})_{\sigma \sigma'}$, is obtained by multiplying the Boltzmann weights of each cell and summing on the indices indicated, namely summing on the central row of sites. The dashed triangle is a Boltzmann weight associated to the three corresponding border sites; it actually introduces an interaction that is fully localized on the border of the lattice. As the actual lattice is just the one formed by the square cells, the triangle has been represented with dashed lines to indicate that is not a lattice cell. The Boltzmann weights associated to one face are

$$W \left(\begin{array}{cc|c} d & c & u \\ a & b & \end{array} \right) = \begin{array}{|c|} \hline u \\ \hline \end{array} = \frac{\sin(\lambda - u)}{\sin \lambda} \delta_{a,c} + \frac{\sin u}{\sin \lambda} \sqrt{\frac{\sin(a\lambda) \sin(c\lambda)}{\sin(b\lambda) \sin(d\lambda)}} \delta_{b,d} \quad (3.2)$$

and those associated to the boundary interactions are

$$B^{r,1} \left(\begin{array}{c|c} r \pm 1 & r \\ r & \end{array} \middle| u, \xi \right) = \begin{array}{c} r \\ \lambda - u \\ \xi \\ r \end{array} = \sqrt{\frac{\sin(r \pm 1)\lambda}{\sin r \lambda}} \frac{\sin(\xi \pm u) \sin(r\lambda + \xi \mp u)}{\sin^2 \lambda} \quad (3.3)$$

where the integers associated to every vertex are called heights and must satisfy the adjacency rule of the Dynkin diagram A_L namely adjacent sites must have height difference of 1 and heights are from 1 to L . I also use a crossing parameter

$$\lambda = \frac{\pi}{L + 1} \quad (3.4)$$

There are more general forms for these weights and also periodic boundary conditions are possible. Here we have chosen those that are more indicated to our development. Indeed, they are critical weights namely they describe the system at its critical temperature. Moreover, the right boundary weight is kept fixed.

In these lattice models the interaction is characterized by the four sites around a face so nearest neighbors and next-to-nearest neighbors interact. On the contrary, in the six-vertex and XXZ models the interaction was between nearest neighbors only. The phase diagram has been studied in [38] by using corner transfer matrix techniques. It is common to call these models from the authors of the paper, ABF models. More precisely, I treat here the A_L models, from the adjacency rules that are used.

These models have a number of useful properties. Indeed, from direct inspection of (3.2) and (3.3) it appears that the transfer matrix is an entire function of the spectral parameter u , that means that its entries are free of poles or other singularities in the whole complex plane.

Transfer matrices at different spectral parameter commute, thus insuring integrability

$$[D(N, u, \xi), D(N, u', \xi)] = 0 \quad (3.5)$$

Indeed, with a standard construction, one can expand in u and generate integrals of motion.

In spite of a different formulation based on faces instead of vertices, the present A_L models are very deeply related to the six-vertex one. The original T-Q relations of Baxter and the six-vertex Bethe ansatz can be modified to hold for the present case.

The double row transfer matrix satisfy a T-Q functional equation that is fully similar to the one that holds in the periodic case (1.37), with small modifications to account for the boundary

$$s(2u) D\left(u + \frac{\lambda}{2}\right) Q(u) = s(2u + \lambda) f\left(u + \frac{\lambda}{2}\right) Q(u - \lambda) + s(2u - \lambda) f\left(u - \frac{\lambda}{2}\right) Q(u + \lambda) \quad (3.6)$$

where I have used

$$f(u) = \left(\frac{\sin u}{\sin \lambda}\right)^{2N}, \quad s(u) = \frac{\sin u}{\sin \lambda} \quad (3.7)$$

The double row transfer matrix is the one in (3.1) but, when not strictly necessary, I omit the dependence by N and ξ .

These expressions hold for a fixed border on the left and the right of (3.1), namely when $r = 1$ and $\tau_0 = r + 1 = 2$. In this case the boundary coupling ξ disappears. Of course, they can be modified to include other cases. The goal here is not to reach the largest generality but to show how the methods work and how the TBA appears in lattice systems. For this reason, I follow the approach of [43] in order to introduce the fusion and the TBA hierarchy.

The new operator $Q(u)$ is a family of matrices that commute each other and commute with the transfer matrix $[Q(u), Q(v)] = [Q(u), D(v)] = 0$. This implies that the same functional equation holds true for the eigenvalues $D(u)$ and $Q(u)$. The eigenvalues of Q are given by

$$Q(u) = \prod_{j=1}^n \frac{\sin(u - u_j) \sin(u + u_j)}{\sin^2 \lambda} \quad (3.8)$$

where u_j are the Bethe roots. The Bethe ansatz equations result by imposing that the transfer matrix is an entire function. Indeed, when $Q(u) = 0$, being $D(u)$ entire, the right hand side must vanish. This forces the following Bethe equations

$$\frac{\sin(2u + \lambda)}{\sin(2u - \lambda)} \left(\frac{\sin(u + \frac{\lambda}{2})}{\sin(u - \frac{\lambda}{2})} \right)^{2N} = -\frac{Q(u + \lambda)}{Q(u - \lambda)} \quad (3.9)$$

It is convenient to shift the transfer matrix

$$\tilde{D}(u) = D(u + \frac{\lambda}{2}) \quad (3.10)$$

With this convention, the transfer matrix is Hermitian in $\text{Re}(u) = 0$. Given the position of its zeros, that will be presented later, the relevant analyticity strip is

$$-\lambda < \text{Re}(u) < \lambda \quad (3.11)$$

Using a standard notation, I let $D(u) = D_0^1$

$$D_k^q = D^q(u + k\lambda), \quad Q_k = Q(u + k\lambda), \quad s_k(u) = s(2u + k\lambda), \quad f_k(u) = (-1)^N s(u + k\lambda)^{2N} \quad (3.12)$$

For “historical” reasons, this notation is customary here: the upper index is not an exponent but just an index. The T-Q relation implies that the eigenvalues $D(u)$ are determined by the eigenvalues $Q(u)$ in the compact form

$$\tilde{D}(u) = \tilde{D}_0 = \frac{s_1 f_{1/2} Q_{-1} + s_{-1} f_{-1/2} Q_1}{s_0 Q_0} \quad (3.13)$$

3.1.1 Fusion hierarchy and TBA hierarchy

From the T-Q relation (3.6) one can construct a hierarchy of models namely a set of transfer matrices D^q recursively defined one after the other. The process, called fusion, was introduced in [39] as a method of obtaining new solutions to the Yang-Baxter equation, by combining R matrices of a known solution. Fusion for the ABF models has been done in [40] and studied in detail in [41], in the case of periodic boundary conditions. The construction holds for the open boundary case for which the fusion has been done in [37]. For what follows, the presence of the hierarchy has very important consequences because it imposes a very particular organization of the zeros of the transfer matrix eigenvalues in the complex plane of the spectral parameter u . At the end, this will lead to “solve” the eigenvalue problem.

From [37], the fusion hierarchy for the transfer matrices is

$$s_{q-2}s_{2q-1}D_0^qD_q^1 = s_{q-3}s_{2q}f_qD_0^{q-1} + s_{q-1}s_{2q-2}f_{q-1}D_0^{q+1}, \quad q = 1, 2, \dots, L-1 \quad (3.14)$$

Notice that the level $q+1$ is extracted from the right hand side, by knowing the levels $q, q-1, 1$. This equation is obtained for the eigenvalues, by extracting the transfer matrix eigenvalue from (3.6) and multiplying by itself after a shift. This procedure is repeated. The second term on the right hand side is the higher fusion level $q+1$ and is fixed by the levels $q, q-1, 1$. This expresses the idea of hierarchy¹. The initial conditions of the recurrence are

$$D_0^{-1} = 0, \quad D_0^0 = f_{-1}I, \quad (3.15)$$

and there is a closure condition: the fusion process is upper limited by L that is the largest value of the “heights” located on the corners of a lattice face

$$D_0^L = 0 \quad (3.16)$$

This fusion makes sense because the obtained higher fusion level transfer matrices still have the remarkable properties of the original $q=1$ transfer matrix. Indeed, they are entire functions and they commute each other. This last property implies that they all have the same set of eigenvectors. Then, they can be interpreted as transfer matrices of new lattice models.

Starting with the fusion hierarchy (3.14), one can use induction to derive the T-system of functional equations [44, 37]

$$s_{q-2}s_qD_0^qD_1^q = s_{-2}s_{2q}f_{-1}f_qI + s_{q-1}^2D_0^{q+1}D_1^{q-1}, \quad q = 1, 2, \dots, L-1 \quad (3.17)$$

For $q=1$, the rightmost term vanishes because of the initial conditions and what remains is just an inversion identity. If we further define

$$d_0^q = \frac{s_{q-1}^2D_1^{q-1}D_0^{q+1}}{s_{-2}s_{2q}f_{-1}f_q}, \quad q = 1, 2, \dots, L-2 \quad (3.18)$$

then the inversion identity hierarchy (T-system) can be put in the form of a Y-system [44, 37]

$$d_0^q d_1^q = (I + d_0^{q+1})(I + d_1^{q-1}) \quad (3.19)$$

with closure

$$d_0^0 = d_0^{L-1} = 0 \quad (3.20)$$

For later convenience, I define the shifted transfer matrices

$$\tilde{D}^q(u) = D^q\left(u + \frac{2-q}{2}\lambda\right), \quad \tilde{d}^q(u) = d^q\left(u + \frac{1-q}{2}\lambda\right) \quad (3.21)$$

¹It is helpful to read all these expressions by just ignoring all the coefficients, namely the factors s_q and f_q .

so that the Y -system takes now the form

$$\tilde{d}^q(u - \frac{\lambda}{2}) \tilde{d}^q(u + \frac{\lambda}{2}) = (1 + \tilde{d}^{q-1}(u))(1 + \tilde{d}^{q+1}(u)) \quad (3.22)$$

The transfer matrices are entire functions of u and periodic

$$D^q(u) = D^q(u + \pi), \quad \tilde{d}^q(u) = \tilde{d}^q(u + \pi) \quad (3.23)$$

They also are real if u is real and satisfy a “crossing symmetry”

$$D^q(u) = D^q((2-q)\lambda - u), \quad d^q(u) = d^q((1-q)\lambda - u) \quad (3.24)$$

The advantage of the shifting these matrices is that the shifted matrices have the same analyticity strip

$$-\lambda < \text{Re}(u) < \lambda \quad (3.25)$$

that means that within a periodicity strip $(\text{Re}(u), \text{Re}(u) + \pi)$ we will use only the analyticity strip (3.25) to solve for the eigenvalues. This choice is related to the position of the zeros and will be presented later.

Lastly, the asymptotic values $\tilde{d}^q(+i\infty)$ were computed in [44]

$$\tilde{d}^q(+i\infty) = \frac{\sin[q\theta] \sin[(q+2)\theta]}{\sin^2 \theta} = \frac{\sin^2(q+1)\theta}{\sin^2 \theta} - 1, \quad \theta = \frac{s\pi}{L+1} \quad (3.26)$$

Functional equations as the T-system and Y-system hold for the periodic boundary case, the open case, and off-criticality. They are a true feature of the this type of lattice models. The same hierarchy holds for the six-vertex model but it is unlimited so there is no truncation.

Notice that my goal is to find the eigenvalues of the nonfused double row transfer matrix $D(u)$. The T-Q relation (3.6) offers us one way: solve the Bethe equations (3.9), put the Bethe roots in (3.8) and use (3.6) to find the eigenvalues $T(u)$. The fusion hierarchy offers another path: solve the whole family of TBA functional equations (3.22) at all orders of fusion; this gives $\tilde{d}^1(u)$ that appears as the rightmost term in (3.17) when $q = 1$ then this equation can be inverted to find $D^1(u) = D(u)$, as wanted. The two paths, albeit mathematically equivalent, offer different levels of difficulty. Solving or at least classifying all solutions of the Bethe equations can be an hard task, given that Bethe roots are complex numbers. It turns out that it is simpler, in this case, to follow the second approach. This will require to control the zeros of the fused transfer matrices.

3.1.2 Functional equations: Y-system, TBA

In the previous section I have presented several systems of functional equations for the transfer matrices. I try now to motivate their relevance in relation to the Zamolodchikov approach to thermodynamic Bethe ansatz.

The Y-system in the form (3.22) can also be written as

$$\tilde{d}^q(u - \frac{\lambda}{2}) \tilde{d}^q(u + \frac{\lambda}{2}) = \prod_r (1 + \tilde{d}^r(u))^{A_{qr}} \quad (3.27)$$

where $A_{qr} = \delta_{q,r-1} + \delta_{q,r+1}$ is the incidence matrix of the Dynkin diagram A_{L-2} . This equation has now the form of the one obtained by Zamolodchikov in [45] for the RSOS scattering theories. These theories are obtained by perturbing a unitary conformal field theory of the minimal series (1.49) by the operator $\phi_{1,3}$. This operator is relevant and it preserves integrability namely the perturbed theory is still integrable. There are two possible directions of perturbation, according to the sign of the coupling. One gives rise to a massive model $A_m^{(-)}$ whose scattering matrix factorizes according to the factorization theorem discussed in the Introduction. The other direction of the perturbation gives a massless theory

$A_m^{(+)}$. The name of “RSOS theories” for these models come from the fact that their two particle scattering matrix, apart overall factors, is the R-matrix of the ABF models of [38], that are also called RSOS.

For these theories in the massive regime, Zamolodchikov wrote the thermodynamic Bethe ansatz equations in [45] for the ground state and showed that they are particular solutions of a Y-system with the same structure of (3.27). The approach of Zamolodchikov does not describe excitations above the ground state but it is reasonable to imagine that the Y-system, more that the thermodynamic Bethe ansatz, describes the symmetries of the model and all its excited states. Y-systems emerge in most (or possibly all) the thermodynamic Bethe ansatz equations that have been derived: see [46] but also one of 135 citations to it, for example [47], that is a recent review on the integrability in AdS/CFT, containing many recent citations to Y-systems.

Now, it is curious to see if the Y-system can emerge, in field theory, in a direct way that avoids the tortuous method of [45]. Indeed, in the series of papers opened with [48], the authors formulated a continuum version of the transfer matrix, of the T-Q relation and of the subsequent functional equations for the minimal series $\mathcal{M}_{2,2n+3}$. This latter is a family of non-unitary conformal field theories with central charge $c = 1 - 3\frac{(2n+1)^2}{2n+3}$. The formulation has been also modified in [49] to describe the perturbation by the operator $\phi_{1,3}$. So, the Y-systems can be obtained constructively from the conformal field theory operators, at the critical point and off criticality.

3.1.3 Zeros of the eigenvalues of the transfer matrix

The conclusion of section 3.1.1 was an indication to solve the Y-system (3.22) to obtain the eigenvalues of the transfer matrix. Before engaging in this calculation, one has to know the analytic properties of the transfer matrices, especially in relation to zeros (and poles, if any).

The eigenvalues $\tilde{D}^q(u)$ of the transfer matrices have many zeros in the complex plane. They can be easily counted from (3.1), considering that each face contributes with a trigonometric term $\sin(a + u)$ (with some a) and the triangular face with two such terms. This means that $\tilde{D}^q(u)$ is a polynomial in $z = \exp(iu)$ and $\bar{z} = \exp(-iu)$ of degree $2N + 2$ so we have to expect $4N + 4$ zeros in a periodicity strip. This counting can be slightly different in presence of other boundary conditions.

Many analytical and numerical observations, and also the “string hypothesis” formulated in [41] for the Bethe roots, indicate that the zeros have a peculiar structure within the strip indicated in (3.25) as analyticity strip. Indeed, zeros can be on the middle axis of the strip, such that their real part vanishes

$$\text{Re}(u) = 0 \tag{3.28}$$

(these are called 1-strings) or on the border of the strip. In that case they appear as pairs

$$\text{Re}(u_1) = -\text{Re}(u_2) = \lambda, \quad \text{Im}(u_1) = \text{Im}(u_2) \tag{3.29}$$

and are called 2-strings, in the usual Bethe ansatz meaning of “string”. This pattern holds for all transfer matrices, with $q = 1, 2, \dots, L - 2$. The matrix \mathbf{D}^{L-1} is proportional to the identity so its strip is empty. Moreover, these are always simple zeros, because Bethe roots are mutually exclusive.

Numerical examples showing this peculiar behaviour of 1- and 2-strings have been presented in a number of papers, starting from the one [52] in which the methods were established. This pattern holds in presence of boundary interactions [53], [54] and with off-critical transfer matrices [55], with massive or massless perturbations. In [43] there is a whole “art gallery” of images of the zeros of the transfer matrix eigenvalues for the critical A_5 model with fixed boundaries. In Figure 3.1 there are three examples of states from the tricritical Ising model A_4 . As it has just two levels of fusion, $q = 1, 2$, it has two analyticity strips. The transfer matrices were not shifted so strips are not centered as in (3.25). In the figure, arrows indicate the dynamics of the zeros, namely their displacement after tuning a boundary coupling.

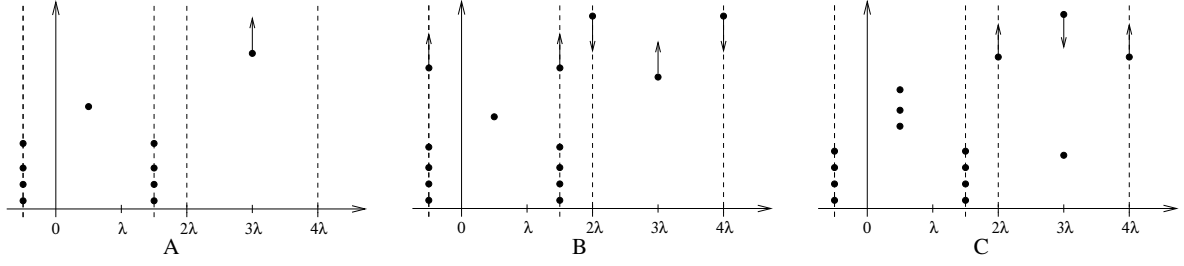


Figure 3.1. Three states for the tricritical Ising model are shown. The arrows indicate three different mechanisms of displacement of the zeros triggered by the change of the boundary coupling constant from one to another conformal boundary condition $\mathcal{B}_{(2,1)} \mapsto \mathcal{B}_{(1,2)}$. Note that this is the reverse of the physical flow which actually goes from the UV point $(1, 2)$ to the infrared point $(2, 1)$. The states are A, $(0|0) \mapsto (0)_+$; B, $(1|0) \mapsto (0)_-$; C, $(0\ 0\ 0|1) \mapsto (0\ 0\ 0|0)_-$. In this image, taken from [54], the shift (3.21) is not used. Strip 1 is on the left, strip 2 on the right.

In some case, often because of the normalization factors in (3.14), some zeros at intermediate positions occur, like

$$\text{Re}(u) = \pm \frac{\lambda}{2} \quad (3.30)$$

I will not consider these cases here. Actually, they do not modify the general ideas that follow, especially because they do not have dynamics: they appear in a fixed number, they show up in all states and have a fixed position.

In addition to (3.28, 3.29), several numerical investigations show that the relative order of the zeros in the $L - 2$ fundamental strips (3.25) is sufficient to identify a common eigenstate of the transfer matrices D^1 to D^{L-2} . Indeed, the state is fixed by the order of appearance of 1- and 2-strings, from the real axis to the asymptotic region. As an example, in Figure 3.1 the state A is given by:

- strip 1: four appearances of 2-strings behind one 1-string
- strip 2: one appearance of 1-string

This means that such an eigenstate is uniquely characterized by a topological information and that the corresponding geometrical data, namely actual positions of zeros, can be inferred by other means. The relative order between different strips has no relevance. Eigenstates/eigenvalues are thus classified by combinatorial rules.

This phenomenon is at the origin of the nomenclature of the states by a set of *non-negative quantum numbers* $\{I_k^{(q)}\}$; considering the upper half-plane, in a strip the lower 1-string carries number 1 and so on counting upward; given the k -th 1-string of strip q , $I_k^{(q)}$ is the number of 2-strings above it. This definition allows an easy reconstruction of the sequence of 1- and 2-strings in the strip (see also Figure 3.1).

Indicating with m_q , n_q the number of 1-strings, 2-strings respectively in strip q (above the real axis), one clearly has

$$n_q \geq I_1^{(q)} \geq I_2^{(q)} \geq \dots \geq I_{m_q}^{(q)} \geq 0 \quad (3.31)$$

It is important to mention that, even if the general scheme proposed here is only true “asymptotically” (large N), deviations are very small and already with a lattice of six faces the general picture appears. Deviations consist in the displacement of the zeros by their asymptotic position (3.28 or 3.29). This phenomenon is also observed in the Bethe ansatz framework: the “string hypothesis” is asymptotic and there are deviations in a finite size lattice.

The number of zeros is expected to grow with the lattice size, according to the counting done at the beginning of this section. Notice first that N grows in steps of 2, because of adjacency rules. Given

a certain set of zeros with their relative order, the addition of an even number of new columns to the lattice has the only effect to add 2-strings to strip 1, near the real axis. In other words, the real axis of the first strip is a source of 2-strings, when N increases. The definition of the quantum numbers has been chosen consistently with this: the quantum numbers of a state do not depend by N . The addition of new 2-strings in the first strip pushes the other zeros (in all strips) far and far from the real axis. This trend is very important for the scaling limit that will be used to get contact with the conformal theory. Indicating a 1-string position by $\frac{i y_k^{(q)}}{L+1}$, the vanishing of the transfer matrix eigenvalue is

$$\tilde{d}^q \left(\frac{i y_k^{(q)}}{L+1} \right) = 0, \quad y_k^{(q)} > 0 \quad (3.32)$$

The leading behaviour with N is

$$y_k^{(q)} = y_k^{(q)}(N) \sim \hat{y}_k^{(q)} + \log N \quad (3.33)$$

where $\hat{y}_k^{(q)}$ is the asymptotic position.

Even if the relative orders and positions of different strips do not matter, there are constraints between the composition of the different strips. They originate in the Y-system and will be presented later.

3.1.4 Solving the Y-system

Aiming at finding the eigenvalues of the transfer matrix, the functional system (3.22) has been “solved” in [52] by taking Fourier transform of the logarithmic derivative. This method requires to control the zeros and poles within the analyticity strip (3.25). After, the method was adapted to several other cases, as in [53] for fixed boundaries, in [54], [56] and [57] for interacting boundaries, in [55] for off-critical lattices and finally in [43] for the whole series of A_L models and for the XXX model. Therefore, there is no need to repeat all the long calculations here.

The final result will be written after taking a scaling limit or continuum limit

$$\hat{d}^q(x) = \lim_{N \rightarrow \infty} \tilde{d}^q \left(N, \frac{i x}{L+1} \right) \quad (3.34)$$

where the matrices of (3.21) are used. The lattice size has been indicated and a new spectral parameter x has been introduced, rotated and dilatated by respect to u^2 . The size N appears in the limit (3.34) first explicitly, counting the number of faces, second implicitly, by the “scaling” positions of the zeros (3.33).

There are two important reasons to require the continuum limit: first, the positions of the zeros in (3.1.3) are “asymptotically” correct therefore exact results can be obtained in the limit only, second because one is usually interested in comparing with conformal field theory data. Conformal field theory is defined on a continuous space, not on the lattice.

From [43], the transfer matrix eigenvalues are

$$-\frac{1}{2} \log D(N, u) = -N \log[\kappa_{\text{bulk}}(u)] - \frac{1}{2} \log[\kappa_{\text{bound}}(u)] - \frac{1}{2} \log \tilde{D}_{\text{finite}}(N, u - \frac{\lambda}{2}) \quad (3.35)$$

where the function κ_{bulk} contains the main bulk contribution and is independent of N , the function κ_{bound} contains a boundary free energy and also is independent of N . These functions are given in [58]; they will not be used here. $\tilde{D}_{\text{finite}}$ is finite for large N but still depends by it and will be given later. The factor $\frac{1}{2}$ has a physical meaning of normalizing to a row-to-row transfer matrix. This produces the following

²Notice that in presence of boundary or bulk interactions, the corresponding parameters usually need to be scaled with N .

lattice partition function³

$$\begin{aligned} Z(N, M, u) &= \text{Tr} (\mathbf{D}(u)^{M/2}) \\ &= \exp \left[-NM \log[\kappa_{\text{bulk}}(u)] - \frac{1}{2}M \log[\kappa_{\text{bound}}(u)] \right] \text{Tr} [\tilde{\mathbf{D}}_{\text{finite}}(N, u - \frac{\lambda}{2})^{M/2}] \end{aligned} \quad (3.36)$$

The solution of the T-system leads to

$$\begin{aligned} & -\frac{1}{2} \log \tilde{D}_{\text{finite}}(N, 0) \\ &= - \int_{-\infty}^{\infty} dy \frac{\log(1 + \tilde{d}^1(N, \frac{iy}{L+1}))}{4\pi \cosh y} - \sum_{k=1}^{m_1} \log \tanh \frac{y_k^{(1)}(N)}{2} + \text{higher order corrections} \\ &= \frac{\pi}{N} E + \text{higher order corrections in } \frac{1}{N} \end{aligned} \quad (3.37)$$

with E independent by N and given by

$$E = -\frac{1}{\pi^2} \int_{-\infty}^{\infty} dy e^{-y} \log(1 + \hat{d}^1(y)) + 2 \sum_{k=1}^{m_1} \frac{1}{\pi} e^{-\hat{y}_k^{(1)}} \quad (3.38)$$

Of course, E depends by the configuration of the zeros in the various strips. I can now express the last factor of the partition function at the isotropic point $u = \frac{\lambda}{2}$ as

$$\chi(\hat{q}) = \text{Tr} [\tilde{\mathbf{D}}_{\text{finite}}(N, 0)^{M/2}] = \sum_{\text{configurations}} \exp \left(-\frac{\pi M}{N} E \right) = \sum_{\text{configurations}} \hat{q}^E \quad (3.39)$$

with

$$\hat{q} = e^{-\frac{\pi M}{N}} \quad (3.40)$$

This \hat{q} is a geometrical parameter that measures the ratio between the number of row and columns in the lattice. When the system is at criticality, the function χ is the conformal partition function. Soon I will make the connection between the “energy” E and conformal energies of the two dimensional conformal theory.

In (3.38), two ingredient are still missing: the transfer matrix \hat{d}^1 and the zeros $\hat{y}_k^{(1)}$. Thanks to the limit (3.34), I can give them an expression. This is not possible before the limit, namely on the lattice, because the positions indicated in section 3.1.3 are only asymptotically correct.

The Y-system provides the missing ingredients by the thermodynamic Bethe ansatz equations

$$\begin{aligned} \log \hat{d}^q(x) &= -4 \delta_{1,q} e^{-x} + \log \prod_{j=1}^{L-2} \prod_{k=1}^{m_j} \left[\tanh \frac{x - \hat{y}_k^{(j)}}{2} \right]^{A_{q,j}} \\ &+ \sum_{j=1}^{L-2} A_{q,j} \int_{-\infty}^{\infty} dy \frac{\log(1 + \hat{d}^j(x))}{2\pi \cosh(x - y)}, \quad q = 1, \dots, L-2 \end{aligned} \quad (3.41)$$

and the quantization conditions

$$\begin{aligned} \hat{\Psi}^q(x) &= 4\delta_{1,q} e^{-x} + i \sum_{r=1}^{L-2} A_{q,r} \sum_{k=1}^{m_r} \log \tanh \left(\frac{x - \hat{y}_k^{(r)}}{2} - i\frac{\pi}{4} \right) \\ &- \sum_{r=1}^{L-2} A_{q,r} \int_{-\infty}^{\infty} dy \frac{\log(1 + \hat{d}^r(y))}{2\pi \sinh(x - y)} \end{aligned} \quad (3.42)$$

$$\hat{\Psi}^q(\hat{y}_k^{(q)}) = \pi n_k^{(q)} = \pi[1 + 2(I_k^{(q)} + m_q - k)] \quad (3.43)$$

³The lattice has M rows and N columns with periodic boundary conditions in the vertical direction and open boundary conditions in the horizontal one, according to (3.1).

where a new family of quantum numbers has been introduced $n_k^{(q)}$. They are odd integers. These two sets of equations close the problem. Indeed by simultaneously solving the TBA equations and the quantization conditions one has the transfer matrices in the center of the strips (3.25) and the position of the zeros. Those with label $q = 1$ enter in the energy expression (3.38) namely in the original transfer matrix eigenvalues. Equations (3.41) and (3.42) are now exact and describe the whole spectrum of the transfer matrix.

The Y-system controls the structure of the equation, namely the appearance of the integral with a difference-like integration kernel and the hyperbolic cosine. The equations still show the full A_{L-2} structure of the Y-system (3.27), in which a strip is coupled with the two neighboring ones. The specific form of the driving term $-4 \delta_{1,q} e^{-x}$ comes from the initial condition for D^0 in (3.15) and indicates how the degrees of freedom with fusion index 1 participate to the energy. The hyperbolic tangent for the zeros and the convolution kernel $1/\cosh(x-y)$ are specific of a critical lattice and they become elliptic functions in the off-critical case. They are mainly fixed by the form of the left side of the Y-system. In presence of boundary interactions, one also adds a specific term as in [56], [57].

The positivity condition

$$1 + \hat{d}^j(x) > 0 \quad (3.44)$$

holds on the whole real axis therefore the integral terms are always real. The zeros terms can produce an imaginary part that corresponds to taking the logarithm of a negative value of $\hat{d}^q(x)$.

The equations (3.41) are legitimately called thermodynamic Bethe ansatz because they correspond to the equations of Zamolodchikov [45] for the RSOS scattering theories. His equations are obtained for the massive case with periodic boundary conditions while here the model is lives on a open strip and the bulk is critical. More importantly, the equations of Zamolodchikov only hold for the ground state while the present lattice approach provides all the states. Notice that the Zamolodchikov equations are usually expresses in terms of the pseudo-energy $\epsilon_q(x) = -\log \hat{d}^q(x)$.

In the general case, there is no explicit solution of this functional equations. For this reason, sometimes numerical solutions were used. It is true that, near a critical regime, it is possible to obtain a closed form for the energy. Indeed, after long calculations, one has a very short form for the conformal energy

$$E = -\frac{c_L}{24} + \frac{1}{4} \mathbf{m}^T C \mathbf{m} + \sum_{q=1}^{L-2} \sum_{k=1}^{m_q} I_k^{(q)} \quad (3.45)$$

where the central charge appears as function of L

$$c_L = 1 - \frac{6}{L(L+1)} \quad (3.46)$$

and $\mathbf{m}^T = (m_1, m_2, \dots, m_{L-2})$ is a vector with the number of 1-strings. In this case, a completely explicit expression for the energies has been obtained. Notice that the solution of the TBA system is still unknown. One arrives at the expression for the energy by manipulation, not by actually solving the TBA or quantization conditions.

In noncritical cases, one can arrive at equations like (3.45) only in the UV and IR limits already described in section 2.2.5 and 2.2.6.

3.2 NLIE versus TBA

Two formalisms have been introduced. One, directly derived from the Bethe ansatz equations, leads to a Klümper-Batchelor-Pearce-Destri-de Vega equation. The other, derived from functional equations for the transfer matrix, leads to the (full spectrum) thermodynamic Bethe ansatz equations. Both produce

one or a system of exact nonlinear integral equations of Fredholm type that allow the evaluation of energy, momenta and other observables. Both equations have the structure

$$\begin{aligned} f(x) &= \nu(x) + \chi(x, \theta_i) + K \star \log(1 + \exp(\alpha f)) \\ \nu(x) &= \text{driving term} \\ \chi(x, \theta_i) &= \text{sources, to be fixed by quantization conditions} \end{aligned} \quad (3.47)$$

with quantization conditions given by

$$f(\hat{\theta} + \theta_i) = I_i, \quad I_i \in \mathbb{Z} \quad (3.48)$$

($\hat{\theta}$ is a fixed shift that appears in the TBA case but not in the DdV one). The function f itself can carry an index, thus participating to a system of coupled equations. The two approaches complement each other, precisely as the T and Q operators complement each other in Baxter T-Q relation (1.37). Indeed, the main message is that the Q operator is behind the Klümper-Batchelor-Pearce-Destri-de Vega approach while the T operator gives rise to the TBA equations.

In spite of the many analogies, the two approaches offer different paths to evaluate the main observables. The choice of using one or the other is mainly dictated by the available initial information: Bethe roots/holes or zeros of the transfer matrix eigenvalues. Notice that the Klümper-Pearce-Destri-de Vega equation is exact in both the finite lattice and the continuum limit while the TBA equations exist only in the continuum limit. Indeed, the first approach does not assume a “string hypothesis” for the zeros/holes while the second one uses the notion that zeros have a fixed real part. This is true in the large size limit and is very much like a “string hypothesis” for the transfer matrices. Actually, it is even more than an hypothesis as it has been widely tested.

Another major difference is in the number of equations. For the sine-Gordon case, one Destri-de Vega equation describes the spectrum. A corresponding TBA set would couple an infinite number of equations. This is better understood if one defines a counting function (see (2.23)) by

$$\mathcal{F} = \exp(iZ(u)) = \frac{Q(u + \lambda)f(u - \frac{\lambda}{2})\sin(u - \lambda)}{Q(u - \lambda)f(u + \frac{\lambda}{2})\sin(u + \lambda)} \frac{\kappa(u)}{\kappa(\lambda - u)} \quad (3.49)$$

such that Bethe equations (3.9) reduce to

$$\mathcal{F}(u_j) = -1 \quad (3.50)$$

The function $\kappa(u)$ is the solution of

$$\begin{aligned} \kappa(u)\kappa(u + \lambda) &= f_1 f_1 s_{-2} s_2 \\ \kappa(u) &= \kappa(\lambda - u) \end{aligned} \quad (3.51)$$

and is given in [58]. This function has mainly a normalization role and is not very important to the present purposes. Notice that in the definition of the counting function the rightmost factor is actually 1. The first case of the T-system (3.17) can be written as

$$1 + d^1(u) = \frac{s_{-1}s_1}{f_1 f_1 s_{-2} s_2} D_0^1 D_1^1 \quad (3.52)$$

therefore, using the T-Q relation (3.6), one gets

$$1 + d^1(u) = \left[1 + \mathcal{F}(u + \frac{\lambda}{2})\right] \left[1 + \frac{1}{\mathcal{F}(u - \frac{\lambda}{2})}\right] \quad (3.53)$$

Now it is obvious that the TBA approach has to solve for the whole hierarchy, here represented by the left hand side, while the counting function of the DdV equation (right hand side) is just related to the

first fusion level. This last equation is very important because it makes the bridge between the two formalisms. Here it has been written for the A_L models but, taking its limit $\lambda \rightarrow 0$ and rescaling u as done in the second part of [43], one adapts it to the XXX model. In that case the hierarchy has no truncation, that means that q is not upper bounded. The six-vertex untruncated hierarchy holds for the sine-Gordon model; this makes clear that the TBA equations for sine-Gordon form an infinite system, as previously indicated. I have derived (3.53) following the paper [64].

The Zamolodchikov scattering formulation of TBA equations [45] was based on a dressed Bethe ansatz, namely a Bethe ansatz based on physical particles and not on quasi-particles; that formulation was not able to treat excited states. An interesting but extremely lengthy method to describe excitations was formulated by Dorey and Tateo [59]. It is based on analytic continuations of the ground state TBA equations by the adimensional parameter $r = MR$, that is the product of the mass of the fundamental particle and of the space size. This parameter enters the TBA equations as

$$\nu(x) = r \cosh x \quad (3.54)$$

and represents the momentum of a particle with (real) rapidity x . Analytic continuation along a path that encloses the singularities of the equation and returns to the real axis produces equations for the excited states: pictorially, moving around branch point singularities let one change the Riemann sheet and access a new excitation level. The difficulty of this approach is in finding systematic classifications of these singularities. Clearly, the lattice formulation given here has no such difficulty and all excitations are easily described.

The work of Bazhanov, Lukyanov and Zamolodchikov [48], [49] was motivated by the need of describing excitations in a more systematic way by constructing a Y-system *ab-initio* for a quantum field theory formulation of transfer matrices and Q operators. They could get the Y-system. The methods shown in this chapter are an efficient way to solve the Y-system, for the ground state and all the excitations.

There is another important difference, in the role of the function $f(x)$. Indeed, in the TBA case $\alpha = -1$, the function $\exp(-f)$ indicates how the energy is distributed among the degrees of freedom and is real, as it is a transfer matrix eigenvalue. In the Klümper-Pearce-Destri-de Vega case, f is a counting function namely it controls the density of Bethe roots (indicated with ρ)

$$\frac{dZ(u)}{du} \sim 2\pi \frac{I_{j+1} - I_j}{u_{j+1} - u_j} \sim 2\pi \rho(u) \quad (3.55)$$

and is especially related to the momenta of the particles. $\alpha = i$ so $\exp(if)$ is a complex function.

3.3 Integrals of motion

The DdV equation and the TBA equations allow the evaluation of energy, momenta and other integrals of motion. For the TBA equations, the equations for high integrals of motion have been obtained in [60] thus providing explicit expressions in the case of the tricritical Ising model with boundary perturbations

$$C_n I_{2n-1}(\xi) = \frac{2}{2n-1} \sum_{k=1}^{m_1} e^{-(2n-1)y_k^{(1)}} + (-1)^n \int_{-\infty}^{\infty} \frac{dy}{\pi} \log(1 + \hat{d}^1(y, \xi)) e^{-(2n-1)y} \quad (3.56)$$

The constant is taken from [48]

$$C_n = 2^{2-n} 3^{1-2n} 5^{1-n} \frac{(10n-7)!!}{n! (4n-2)!} \pi \quad (3.57)$$

The case $n = 1$ gives the energy $E = I_1(\xi)$ as in (3.38). The TBA equations and quantization conditions are as in (3.41) and (3.42) with $L = 4$ and with the addition, on the right hand side of $\log \hat{d}^q(x)$, of the

boundary interaction term $\log g_q(x, \xi)$. In particular, for the boundary flow $(1, 2) \rightarrow (1, 1)$ the choice is

$$g_1(x, \xi) = \tanh \frac{x + \xi}{2}, \quad g_2(x, \xi) = 1 \quad (3.58)$$

with $\xi = -\infty$ corresponding to the boundary condition (1,2), namely an unstable UV point, and $\xi = +\infty$ to the (1,1), a stable IR point. This perturbative flow is triggered by the boundary operator $\phi_{1,3}$, namely by an operator that acts on the border of the strip. Notice also that \hat{t}_1 and \hat{g}_1 of [60] correspond to \hat{d}^2 and \hat{g}_2 of the present paper; analogously \hat{t}_2 and \hat{g}_2 correspond to \hat{d}^1 and \hat{g}_1 . These equations are strategically important to fix the correspondence with basis vectors in the conformal field theory. Indeed, the difficulty with TBA equations is that they provide expressions for the energy but no indication of the states. In conformal field theory, given the high amount of symmetry, typically many states have the same energy. For example, in a standard cylinder quantization, the vacuum sector of the tricritical Ising model has level degeneracies

$$1, 0, 1, 1, 2, 2, 4, \dots \quad (3.59)$$

How can one match lattice states and conformal field theory states? The first few conformal field theory conserved charges are given in [8], obtained after quantization of classical integrals of motion of the modified KdV and sine-Gordon models. This derivation is very important because it is naturally related to $\phi_{1,3}$ perturbations and to the structure of the Y-system (3.22). The integrals of motion are

$$\begin{aligned} I_1 &= L_0 - \frac{c}{24} \\ I_3 &= 2 \sum_{n=1}^{\infty} L_{-n} L_n + L_0^2 - \frac{2+c}{12} L_0 + \frac{c(5c+22)}{2880} \\ I_5 &= \sum_{m,n,p} :L_n L_m L_p: \delta_{0,m+n+p} + \frac{3}{2} \sum_{n=1}^{\infty} L_{1-2n} L_{2n-1} + \sum_{n=1}^{\infty} \left(\frac{11+c}{6} n^2 - \frac{c}{4} - 1 \right) L_{-n} L_n \\ &\quad - \frac{4+c}{8} L_0^2 + \frac{(2+c)(20+3c)}{576} L_0 - \frac{c(3c+14)(7c+68)}{290304} \end{aligned} \quad (3.60)$$

Expressions for the following cases become quickly very complicated. In terms of the generators of the Virasoro algebra, the space of states is built by linear superpositions of the states (1.48). A conceptually simple (but technically very difficult) problem of linear algebra is to find common eigenstates of the integrals of motion on the Virasoro basis (1.48). For the first few levels, an explicit expression has been evaluated in [60], together with the corresponding eigenvalues, providing a list of eigenvalues I_n^{CFT} . At higher energy, the eigenvalues are given by solving algebraic equations of degree equal to the degeneracy.

Using the eigenvalues (3.56), one has another list I_n^{TBA} . Matching the two lists creates a one-to-one dictionary that in [60] was appropriately called *lattice-conformal dictionary*. The wording is inspired from [61]. I'm not aware of closed expressions for the integrals (3.56), like the energy expression (3.45), even if I believe they should exist. For this reason, numerical evaluations have been used. Notice that, even if I_n^{TBA} and I_n^{CFT} are evaluated numerically, the matching is exact because the spectrum is discrete, as one can appreciate looking at the values given for the vacuum sector in table 3.1.

One can wonder about the fate of such integrals of motion when a relevant perturbation is switched on. In the present case, where the $\phi_{1,3}$ boundary perturbation is concerned, the TBA formulation is preserved because, as already discussed, this perturbation generates flows for which the Y-system and the functional equations still hold. This is well known on the lattice side. It is also known that at special points of the sine-Gordon coupling, one describes the $\phi_{1,3}$ perturbations of the minimal models (1.49) therefore it is natural to expect that the quantities (3.60) are compatible with such a perturbation, being derived from the sine-Gordon integrals of motion. Among the possible families of involutive integrals of motion allowed in the CFT, they are those whose ranks (or Lorentz spins, namely the indices n) are predicted to be preserved, by the counting argument in [51]. The perturbed operators are given in [49]. Numerical investigations of $I_3(\xi)$ were done in [60].

Table 3.1. Comparison of the eigenvalues of I_3 and I_5 from conformal field theory and from TBA in the vacuum sector of the tricritical Ising model. The left column contains the level degeneracy (l.d.) as indicated in the conformal character: dq^l

l.d.	lattice-conformal dictionary	I_3 (CFT)	I_3 (TBA)	I_5 (CFT)	I_5 (TBA)
1	$() \longleftrightarrow 0\rangle$	0.0061979	0.0061979	-0.0028301	-0.0028301
$1q^2$	$(00) \longleftrightarrow L_{-2} 0\rangle$	4.2561979	4.2561979	8.1731074	8.1731074
$1q^3$	$(10) \longleftrightarrow L_{-3} 0\rangle$	19.131198	19.131197	104.14545	104.14545
$2q^4$	$(20) \longleftrightarrow 3(\frac{4+\sqrt{151}}{5}L_{-4} + 2L_{-2}^2) 0\rangle$	52.052045	52.052042	556.20159	556.20155
	$(11) \longleftrightarrow 3(\frac{4-\sqrt{151}}{5}L_{-4} + 2L_{-2}^2) 0\rangle$	22.560351	22.560348	108.29650	108.29648
$2q^5$	$(30) \longleftrightarrow (\frac{7+\sqrt{1345}}{2}L_{-5} + 20L_{-3}L_{-2}) 0\rangle$	110.13688	110.13687	1943.8246	1943.8244
	$(21) \longleftrightarrow (\frac{7-\sqrt{1345}}{2}L_{-5} + 20L_{-3}L_{-2}) 0\rangle$	55.125517	55.125511	551.34946	551.34937
$4q^6$	$(40) \longleftrightarrow (11.124748L_{-6} + 9.6451291L_{-4}L_{-2} + 4.4320186L_{-3}^2 + L_{-2}^3) 0\rangle$	200.49775	200.49773	5280.2710	5280.2705
	$(31) \longleftrightarrow (-4.9655743L_{-6} + 2.3354391L_{-4}L_{-2} + 0.71473858L_{-3}^2 + L_{-2}) 0\rangle$	112.78147	112.78146	1919.0972	1919.0969
	$(22) \longleftrightarrow (0.66457527L_{-6} - 1.2909210L_{-4}L_{-2} - 1.2605013L_{-3}^2 + L_{-2}^3) 0\rangle$	69.265146	69.265138	636.39114	636.39101
	$(0000 00) \longleftrightarrow (-1.6612491L_{-6} - 4.0646472L_{-4}L_{-2} + 1.4118691L_{-3}^2 + L_{-2}^3) 0\rangle$	35.980431	35.980428	209.28433	209.28430

The expressions (3.56) actually work for all the other models described by (3.41). I would like to mention that very similar expressions hold in the DdV formalism [62]. Also these authors do not find a closed form for (3.56), except at a free fermion point. In the Ising case A_3 a closed form is known in terms of poly-logarithms [63], but this is a free fermion!

3.4 Numerical considerations

The form of equations (3.47) is particularly suited to be solved by iteration. Indeed, starting from an initial guess

$$f_0 = \nu(x) \quad (3.61)$$

one iterates by

$$f_{k+1}(x) = \nu(x) + \chi(x, \theta_i) + K \star \log(1 + \exp(\alpha f_k)) \quad (3.62)$$

up to the required precision. This looks very easy and, sometimes, it is so. The difficulties come when there are sources to fix, in particular when they are outside the real axis, in which case one experiences also a big increase of the computational time. The difficulty is due to the mixing of the “functional” problem, namely finding a function f , with the “sources” problem, namely finding the sources. Then, one has to iterate at the same time on f and on θ_k .

The numerical approach has been used in many occasions. In [56], there is a wide discussion in relation to the TBA case. See also the paper [67] for the DdV case. Here I would like to discuss about the question of convergence. Is the iteration (3.62) converging? Is it converging to the good solution, if there are multiple solutions?

The *contraction mapping theorem* states that if a mapping $\mathcal{M} : V \rightarrow V$ on a complete metric space V is a contraction then there exists a unique fixed point $f_0 = \mathcal{M}(f_0)$ and all the sequences obtained under iteration starting from an arbitrary initial point $f \in V$ converge to the fixed point. In practice, the derivative $|\mathcal{M}'(f)|$ measures the strength of the contraction and the rate of convergence. The case $|\mathcal{M}'(f)| < 1$ is a contraction while $|\mathcal{M}'(f)| > 1$ is a dilatation. Values close to 0 converge quickly, values close to 1 converge slowly.

If one could show that the mapping $f_{k+1} = \mathcal{M}(f_k)$ is a contraction, then the answer to the previous questions would be affirmative. Unfortunately, the mapping is not easy to evaluate. Restricting to the TBA case, one can do some steps forward. By varying f in (3.62) one has

$$\delta f_{k+1}(x) = \int \frac{1}{2\pi \cosh(x-y)} \frac{-\exp(-f_k)}{1 + \exp(-f_k)} \delta f_k(y) dy \quad (3.63)$$

By the integral

$$\int_{-\infty}^{\infty} \frac{1}{\cosh t} dt = \pi,$$

the first fraction sums up to $\frac{1}{2}$ therefore “in average” is a contraction. If f_k is real, as it happens in the ground state, the last fraction has absolute value lower than 1. This suggests that the integration acts globally as a contraction with factor smaller than $\frac{1}{2}$ therefore iteration is convergent to the unique solution.

Numerical calculations have shown that, in absence of sources, the convergence of the iteration equations is usually fast. In the $L = 4$ case, namely the tricritical Ising model, 30 iterations are sufficient to reach 9 significant digits, that confirms the estimate of a contraction factor of $1/2$

$$2^{-30} \sim 10^{-9} \quad (3.64)$$

In presence of sources, the intuitive evaluation breaks down because one has to iterate on the sources position. This is related to the fact that f_k can acquire an imaginary part multiple of π , although $1 + \exp(-f) > 0$ as in (3.44). On numerical calculations, one immediately observes the need to iterate

longer, up to hundred times when several sources are considered. Moreover, in [56] it was pointed out that certain algorithms to fix sources do not converge. The problem does not appear for the function f itself. When algorithms for sources do not converge, they appear to be dilatations, in which case the iteration takes away from the fixed point and the solution must be found by other means. This fact is curious and could become more serious in other models with different kernel or sources structure, up to the point of preventing the unicity of the solution.

In the models considered here, an incomplete possible argument goes as follows. In (3.42) one neglects the integrals, that often appear to be much smaller than the source terms. Then, an equation with $q > 1$ looks like

$$\exp(-i \pi n_k^{(q)}) = \prod_{j=1}^{m_{q-1}} \tanh\left(\frac{\hat{y}_k^{(q)} - \hat{y}_j^{(q-1)}}{2} - i\frac{\pi}{4}\right) \prod_{h=1}^{m_{q+1}} \tanh\left(\frac{\hat{y}_k^{(q)} - \hat{y}_h^{(q+1)}}{2} - i\frac{\pi}{4}\right) \quad (3.65)$$

and $\hat{y}_k^{(q)}$ can be extracted for example by

$$\tanh\left(\frac{\hat{y}_k^{(q)} - \hat{y}_1^{(q-1)}}{2} - i\frac{\pi}{4}\right) = Y(\hat{y}_k^{(q)}) \quad (3.66)$$

$$Y(\hat{y}_k^{(q)}) \stackrel{\text{def}}{=} \exp(-i \pi n_k^{(q)}) \prod_{j=2}^{m_{q-1}} \coth\left(\frac{\hat{y}_k^{(q)} - \hat{y}_j^{(q-1)}}{2} - i\frac{\pi}{4}\right) \prod_{h=1}^{m_{q+1}} \coth\left(\frac{\hat{y}_k^{(q)} - \hat{y}_h^{(q+1)}}{2} - i\frac{\pi}{4}\right) \quad (3.67)$$

Notice that $Y()$ is a function of modulus one. Inverting the tanh leads to the iterative form

$$\hat{y}_k^{(q)} = \hat{y}_1^{(q-1)} + i\frac{\pi}{2} + \log \frac{1 + Y(\hat{y}_k^{(q)})}{1 - Y(\hat{y}_k^{(q)})} = \mathcal{Y}_k^{(q)}(\hat{y}_k^{(q)}) \quad (3.68)$$

The derivative is

$$\frac{d\mathcal{Y}_k^{(q)}}{d\hat{y}_k^{(q)}} = \frac{2Y'(\hat{y}_k^{(q)})}{1 - (Y(\hat{y}_k^{(q)}))^2} \quad (3.69)$$

If this derivative is larger than 1, (3.68) becomes a dilatation. Evaluating it is not easy. If the sources can be arranged in such a way that $Y(\hat{y}_k^{(q)})$ is sufficiently close to ± 1 , the denominator can be made close to zero. This probably means that the derivative can be quite large and be a dilatation, but this analysis is not conclusive. Several numerical investigations have shown that there are sources arrangements where iterative algorithms as (3.68) do not converge at all. In these cases, other methods are needed. For example, one first estimates the interval in which the source is expected then locates it by the bisection method. Of course, this uses much more computer time than an iterative method.

In [56] a similar situation was described in relation to a boundary function $g(x, \xi)$. The treatment given here is complementary to that one and, in some sense, is more general because it does hold even when boundary parameters are absent.

In the frame of the DdV equation, in [29] and [32] the case of “special holes” was left unsolved: in that case, the functional equation itself seems to fail to converge, or better, it converges to a nonsense, possibly for the reasons indicated here.

The lesson of this analysis is that iterations can give rise to unexpected problems and this could have consequences about the unicity of the solution. On the other hand, in my numerical TBA calculations, I never observed problems of unicity.

3.5 Discussion

I have introduced the thermodynamic Bethe ansatz method, sketched its lattice derivation and discussed the relevance of the Y-systems to summarize the symmetries of the model. I have presented the integrals

of motion. The methods of DdV and TBA have been compared and numerical considerations have been shown.

Personally, I have worked on TBA equations for a fair amount of time (2000 to 2006). My contribution has been important.

- I have derived and treated TBA equations for the boundary flows of the tricritical Ising model.
- I have established the lattice-conformal dictionary.
- I extended the TBA to all A_L models and also to the XXX model.
- I analyzed how the zeros move in consequence of boundary flows.
- I derived the conformal characters (conformal partition functions) from TBA.
- I have done extensive high precision numerical calculations with TBA equations, in presence of many sources and of several coupled equations.
- I worked on the physical combinatorics of quasi-particles. They form a lattice gaz whose partition function is the conformal character.

The first development that I propose is to make systematic the lattice-conformal dictionary. This is probably related to the realization of a lattice Virasoro algebra. It will lead to a better understanding of the space of states.

The second is related to the quasi-particles and the physical combinatorics. I have already experimented, in [65], algebraic formalisms to express these quasi-particles. The formulation was primitive but other authors worked on it and proposed more effective formalisms, see [66] and the papers that followed it. I think the clarification of an algebraic formalism for the quasi-particles would help to work on the space of states of the minimal models and their perturbations.

Chapter 4

Hubbard model and integrability in $\mathcal{N} = 4$ SYM

The Hubbard model was introduced in order to investigate strongly correlated electrons in matter [68, 69] and since, it has been widely studied, essentially due to its connection with condensed matter physics. It has been used to describe the Mott metal-insulator transition [70, 71], high critical temperature T_c superconductivity [72, 73], band magnetism [74] and chemical properties of aromatic molecules [75]. The literature on the Hubbard model being rather large, I refer to the books [76, 77] and references therein. Exact results have been mostly obtained in the case of the one-dimensional model, which enters the framework of our study. In particular, the 1D model Hamiltonian eigenvalues have been obtained by means of the coordinate Bethe Ansatz by Lieb and Wu [78].

One of the main motivations for the present study of the Hubbard model and its generalisations is the fact that it has unexpectedly appeared in the context of $N = 4$ super Yang-Mills theory. This is a superconformal gauge theory in four dimensions, conjectured to be dual to a string theory in a $\text{AdS}_5 \times \text{S}^5$ background, a ten dimensional space.

Indeed, it was noticed in [79] that the Hubbard model at half-filling, when treated perturbatively in the coupling, reproduces the long-ranged integrable spin chain of [82] as an effective theory. It thus provides a localisation of the long-ranged spin chain model and gives a potential solution to the problem of describing interactions which are longer than the length of the spin chain. The Hamiltonian of this chain was conjectured in [82] to be an all-order description of the dilatation operator of $N = 4$ super Yang-Mills in the $SU(2)$ sector. That is, the energies of the spin chain were conjectured to be proportional to the anomalous dimensions of the gauge theory operators in this sector. After, it was shown that starting with the fourth loop terms, the Hubbard model is incomplete in describing the dilatation operator [80], certain highly nontrivial phase factors being required. But this wasn't the end of the story! The full factorized scattering matrix of the gauge theory has been studied and Beisert has shown the relation of this S-matrix with the Shastry R-matrix of the Hubbard model [81]. This means that the integrable structure of the Hubbard model enters in the conjectured integrable structure of the SYM theory.

In this chapter, I will present two different approaches to the Hubbard model, one based on the Klümper-Batchelor-Pearce-Destri-de Vega method [96, 67] and one based on R-matrices [94]. The first one has led to the evaluation of energies for the antiferromagnetic state. It allows also to control the order of the limits of high coupling and high lattice size. The large size of the model is easily treated at all values of the coupling. This is important as in the SYM frame it corresponds to very long monomials of local operators, totally inaccessible with ordinary diagrammatic techniques. For the second approach, in 2005-2006 I thought there may be the possibility that some integrable extension of the Hubbard model could be put in relation to other subsectors of the $N = 4$ super Yang-Mills theory given that the Hubbard model itself was observed in relation to the sector $SU(2)$. Here I will discuss a general approach to construct a number of supersymmetric Hubbard models. Each of these models can be treated perturbatively and thus gives rise to an integrable long-ranged spin chain in the high coupling limit.

Other symmetric or supersymmetric generalizations of the Hubbard model have been constructed, see e.g. [93]. These approaches mainly concern high T_c superconductivity models. They essentially use the $gl(1|2)$ or $gl(2|2)$ superalgebras, which appear as the symmetry algebras of the Hamiltonian of the model. The approach I have adopted in [94] however is different, being based on transfer matrices and quantum inverse scattering framework. It ensures the integrability of the model and allows one to obtain local Hubbard-like Hamiltonians for general $gl(N|M)$ superalgebras. After a Jordan-Wigner transformation, these Hamiltonians appear to describe one or more families of charged and chargeless fermions.

4.1 The Hubbard model

The Hubbard model, introduced in [68, 69], describes hopping electrons on a lattice, with an ultralocal repulsive potential that implements a screened Coulomb repulsion, with $U > 0$. The 1-dimensional Hamiltonian is given by

$$H = -t \sum_{i=1}^L \sum_{\rho=\uparrow,\downarrow} \left(e^{i\phi} c_{\rho,i}^\dagger c_{\rho,i+1} + e^{-i\phi} c_{\rho,i+1}^\dagger c_{\rho,i} \right) + U \sum_{i=1}^L (1 - 2n_{\uparrow,i})(1 - 2n_{\downarrow,i}) \quad (4.1)$$

where c, c^\dagger are usual fermionic operators, i indicates the lattice site and ρ is the “spin orientation”. I will always use periodic boundary conditions.

The physical idea behind this Hamiltonian is that the metallic positive ions create the crystalline structure. Each ion puts up to two electrons in the conductive band. Ions are much heavier than electrons so for most investigations they can be considered as static thus the lattice has no dynamics. Electrons in the conductive band repel each other (of course!) but they also experience major screening effects. Indeed, an electron feels the repulsion of the other electrons but also the strong, periodic, attraction by the ions. This makes the Coulomb repulsion short-ranged. In the Hubbard model, the electronic repulsion is modeled with an ultralocal term: electrons interact only if they are on the same site. Pauli exclusion then implies that they interact if they have opposite spin only. Pauli exclusion implies also that a maximum of $2L$ electrons can be accommodated in the lattice, in which case it is “fully filled”. I will often use the “half filled” case that contains precisely L electrons. The phase ϕ in the Hamiltonian represents a uniform magnetic field. For many purposes, one can put it to zero. In the approach of [67] this phase was introduced to fit with the Hubbard model used in [79].

There are some features that can be explored without too much calculative effort. If $U = 0$, the Hamiltonian describes free fermions (electrons). The first term in (4.1) describes hopping between nearest neighbor sites in such a way that electrons can freely move around, yielding a conductor. On the other hand, when U becomes very large, it appears that the total energy is lower if one can make negative the contribution from the potential term $(1 - 2n_{\uparrow,i})(1 - 2n_{\downarrow,i})$, namely if on each site there is just one electron. At half filling and large U , the ground state has precisely this form with one electron per site, no empty sites and no doubly occupied sites. At zero temperature and large U this state is fully frozen because overturning a spin would require an amount of energy of U to create a state with a doubly occupied site. This “frozen” state describes a Mott insulator namely a system whose conductive band is not empty but the Coulomb interaction forbids any electronic displacement. At positive temperature, the ground state is always conductive because thermal excitations can provide the amount of energy needed to create vacancies and double occupancies.

The large U regime is the spin chain limit. Indeed, the Hubbard model looks very close to an Heisenberg XXX model: one (quantum) spin per site, up or down. Notice that if the lattice is not half filled, there is conduction whatever is the value of U .

The underlying algebraic structure leads to superalgebras. In a first instance, I consider a single fermion

$$\{c, c^\dagger\} = \mathbf{I}, \quad n = c^\dagger c \quad (4.2)$$

where \mathbf{I} is the identity operator, n is the number operator and $\{, \}$ is the anticommutator. The operators $c, c^\dagger, \mathbf{I}, n$ form a realization of a $gl(1|1)$ superalgebra. One way to see this is to write down the whole set of “commutation rules”

$$[n, c] = -c, \quad [n, c^\dagger] = c^\dagger, \quad [X, \mathbf{I}] = 0 \text{ for } X \in \{n, c, c^\dagger\} \quad (4.3)$$

These and (4.2) can be realized by the two dimensional matrices of $gl(1|1)$

$$E_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = c, \quad E_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = c^\dagger, \quad E_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = n, \quad E_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = \mathbf{I} - n.$$

On each site of the Hubbard lattice there are two “spin polarizations” so on each site there is a $gl(1|1) \oplus gl(1|1)$ superalgebra and, on the whole lattice, the fermionic structure

$$\{c_{\rho,i}, c_{\rho',j}^\dagger\} = \delta_{\rho,\rho'} \delta_{i,j} \quad \{c_{\rho,i}, c_{\rho',j}\} = \{c_{\rho,i}^\dagger, c_{\rho',j}^\dagger\} = 0 \quad (4.4)$$

is L -times the tensor product of the one site structure. I can easily represent the fermionic structure by a graded tensor product of the matrices

$$E_{12;\rho,i} = c_{\rho,i}, \quad E_{21;\rho,i} = c_{\rho,i}^\dagger, \quad E_{22;\rho,i} = n_{\rho,i} = c_{\rho,i}^\dagger c_{\rho,i}, \quad E_{11;\rho,i} = 1 - n_{\rho,i} = c_{\rho,i} c_{\rho,i}^\dagger \quad (4.5)$$

When it occurs, the second pair of labels ρ, i indicates the spin polarization ρ and the site i . The matrices E_{12}, E_{21} are taken of fermionic character (they satisfy anticommutation relations whatever their spin and space labels are) and E_{11}, E_{22} are taken of bosonic character (they always enter commutation relations whatever their spin and space labels are). The relation (4.5) is a graded Jordan-Wigner transformation¹ and respects periodic boundary conditions². I now rewrite the Hubbard Hamiltonian in the matrix language

$$H = -t \sum_{i=1}^L \sum_{\rho=\uparrow,\downarrow} (E_{21;\rho,i} E_{12;\rho,i+1} + E_{21;\rho,i+1} E_{12;\rho,i}) + U \sum_{i=1}^L (E_{11;\uparrow,i} - E_{22;\uparrow,i})(E_{11;\downarrow,i} - E_{22;\downarrow,i}) \quad (4.6)$$

and I split it into the sum of the two polarizations

$$H = H_{XX}^\uparrow + H_{XX}^\downarrow + U \sum_{i=1}^L (E_{11;\uparrow,i} - E_{22;\uparrow,i})(E_{11;\downarrow,i} - E_{22;\downarrow,i}); \quad (4.7)$$

$$H_{XX}^\rho = -t \sum_{i=1}^L (E_{21;\rho,i} E_{12;\rho,i+1} + E_{21;\rho,i+1} E_{12;\rho,i}).$$

Taking one polarization of the kinetic term one easily sees

$$E_{21;\rho,i} E_{12;\rho,i+1} + E_{21;\rho,i+1} E_{12;\rho,i} = \frac{1}{2} [E_{x;\rho,i} E_{x;\rho,i+1} + E_{y;\rho,i} E_{y;\rho,i+1}] \quad (4.8)$$

$$E_{x;\rho,i} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_{\rho,i}, \quad E_{y;\rho,i} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_{\rho,i}$$

the appearance of two (graded) XX spin chain Hamiltonians³, one for each polarisation, within the Hubbard model.

¹The ordinary Jordan-Wigner transformation is $c_{\uparrow,i}^\dagger = \sigma_{\uparrow,i}^- \prod_{k>i} \sigma_{\uparrow,k}^z$ for the up polarization; an additional term occurs for the down polarisation.

²The standard one violates periodicity.

³At this point it should be clear that the difference between graded and non graded cases appears when boundary effects are observed; the thermodynamic limit usually ignores such terms, being sensitive to bulk contributions only.

It turns out that the breaking of (4.7) into the Hamiltonian of two XX models plus a potential term allows one to generalise this model to higher algebraic structures by maintaining integrability⁴.

Exact investigations on the Hubbard model required many years of work. A first hint of integrability came from the coordinate Bethe Ansatz solution obtained by Lieb and Wu [78] in 1968 but a full understanding of it by an R-matrix satisfying a Yang-Baxter equation came much later. An R-matrix was first constructed by Shastry [83, 84] and Olmedilla et al. [85], by coupling the R-matrices of two independent XX models, through a term depending on the coupling constant U of the Hubbard potential. The proof of the Yang-Baxter relation for the R-matrix was given by Shiroishi and Wadati [86] in 1995.

The construction of the R-matrix was then generalised to the $gl(N)$ case by Maassarani et al., first for the XX model [87] and then for the $gl(N)$ Hubbard model [88, 89]. Later, I will use this approach to generalize to $gl(N|M)$ models.

The Lieb-Wu equations [78, 79] for the Hubbard model are, in the half-filling case,

$$e^{i\hat{k}_j L} = \prod_{l=1}^M \frac{u_l - \frac{2t}{U} \sin(\hat{k}_j + \phi) - \frac{i}{2}}{u_l - \frac{2t}{U} \sin(\hat{k}_j + \phi) + \frac{i}{2}}$$

$$\prod_{j=1}^L \frac{u_l - \frac{2t}{U} \sin(\hat{k}_j + \phi) + \frac{i}{2}}{u_l - \frac{2t}{U} \sin(\hat{k}_j + \phi) - \frac{i}{2}} = \prod_{\substack{m=1 \\ m \neq l}}^M \frac{u_l - u_m + i}{u_l - u_m - i}, \quad (4.9)$$

where M is the number of down spins; here they are modified to include the phase. The spectrum of the Hamiltonian is then given in terms of the momenta \hat{k}_j by the *dispersion relation*

$$E = -2t \sum_{j=1}^L \cos(\hat{k}_j + \phi). \quad (4.10)$$

Starting from these “Bethe equations”, I will present two coupled nonlinear integral equations for the antiferromagnetic state of the model. These equations are derived in [67] in the same framework of the Klümper-Batchelor-Pearce-Destri-de Vega approach of the chapter 2.

For reason of completeness, it is important to point out that the thermodynamics (infinite length L , but finite temperature) of the Hubbard model has been studied in [90, 91] by means of three nonlinear integral equations. This approach was based on the equivalence of the quantum one-dimensional Hubbard model with the classical two-dimensional Shastry model. The work presented here was oriented to gauge theory understanding. The objective was to obtain energies of the Hubbard model at zero temperature but at any value of the lattice size L therefore the approach of [90, 91] was not appropriate.

There are some features of (4.9) that deserve some attention. In the large coupling limit (large U), the second set of equations decouples from the first one and coincides with the XXX Bethe equations (1.41), once the limit $\lambda \rightarrow 0$ has been taken. This is consistent with the argument, given earlier, that the spin chain limit of the Hubbard model is the XXX model. On the opposite, if $U = 0$ the second group becomes useless because the first group is enough to fix \hat{k}_j and the energy. The first group reduces to

$$e^{i\hat{k}_j L} = 1 \quad (4.11)$$

that is the box quantization of free particles. The momenta are all different, as usual in Bethe ansatz, therefore particles are fermions. Indeed, in this limit the Hamiltonian describes free fermions.

From this analysis, one can see that the Lieb-Wu equations describe the phenomenon of spin-charge separation. Indeed, the momenta \hat{k}_j are as many as the electrons so they carry charge. Instead, the “rapidities” u_ℓ are as many as the down spins so they carry spin. In the spin limit the quasiparticles described by \hat{k}_j disappear from the equations while at the free fermion point $U = 0$ it is the opposite.

⁴The flux ϕ does not affect integrability properties.

4.1.1 $\mathcal{N} = 4$ super Yang-Mills and AdS/CFT

This superconformal field theory in its planar limit, namely the limit of an infinite number of colors, is probably an integrable theory. It seems related to the Hubbard model, as it was first observed in [79]. The following relation between coupling constants was proposed

$$\frac{t}{U} = \frac{g}{\sqrt{2}} = \frac{\sqrt{\lambda}}{4\pi^2}, \quad U = -\frac{1}{g^2} = -\frac{8\pi^2}{\lambda} \quad (4.12)$$

where λ is the 't Hooft coupling of the theory and g is related to the SYM coupling. The Hubbard lattice must be taken half-filled. The energy (4.10) is related to the anomalous dimensions γ_{SYM} of the super Yang-Mills operators in the scalar sector $SU(2)$ by

$$\gamma_{\text{SYM}} = \frac{\lambda}{8\pi^2} E \quad (4.13)$$

The lattice size L is identified with the “length” of the operators in terms of the fundamental scalar fields of the theory.

This theory is believed to be dual to a type II string theory on a $AdS_5 \times S^5$ background. This and other dualities between quantum field theory and string theory are known as AdS/CFT dualities, after Maldacena [97]. The duality has a very nice and curious feature: it exchanges strong and weak couplings. As strong coupling calculations are usually difficult, the duality makes them accessible *via* weak coupling calculations in the dual theory.

After the important work of Minahan and Zarembo [17], there has been an explosion of researches in this domain. The AdS/CFT duality has been enriched of tools and new calculation methods by recognizing that there are integrable models, on both sides of the duality.

4.2 Universal Hubbard models

Following the methods of [87] and [92], it has been possible to generalize the Hubbard model to include more general symmetries than the original $SU(2)$ one. In a first stage, the XX model is generalized to (almost) arbitrary vector spaces and symmetries. Secondly, two copies of the XX model are “glued” to form a Hubbard model. This is the usual construction of the R-matrix of the Hubbard model.

I will use the standard notation in which the lower index indicates the space on which the operator acts. For example, to $A \in \text{End}(V)$, I associate the operator $A_1 = A \otimes \mathbf{I}$ and $A_2 = \mathbf{I} \otimes A$ in $\text{End}(V) \otimes \text{End}(V)$. More generally, when considering expressions in $\text{End}(V)^{\otimes k}$, A_j , $j = 1, \dots, k$ will act as the identity in all spaces $\text{End}(V)$ except the j^{th} one.

To deal with superalgebras, I will also need a \mathbb{Z}_2 grading $[\cdot]$ on V , such that $[v] = 0$ will be associated to bosonic states and $[v] = 1$ to fermionic ones.

The construction of a universal XX model is mainly based on general properties of projectors and permutations. The needed projectors $\pi, \tilde{\pi}$ select a proper subspace of V

$$\pi : V \rightarrow W, \quad \tilde{\pi} = \mathbf{I} - \pi : V \rightarrow \widetilde{W} \quad \text{with} \quad V = W \oplus \widetilde{W} \quad (4.14)$$

In the tensor product of two vector spaces I take the possibly graded permutation

$$P_{12} : \begin{cases} V \otimes V \rightarrow V \otimes V \\ v_1 \otimes v_2 \rightarrow (-1)^{[v_1][v_2]} v_2 \otimes v_1 \end{cases} \quad (4.15)$$

and also Σ_{12}

$$\Sigma_{12} = \pi_1 \tilde{\pi}_2 + \tilde{\pi}_1 \pi_2 \quad (4.16)$$

It is easy to show that Σ_{12} is also a projector in $V \otimes V$: $(\Sigma_{12})^2 = \Sigma_{12}$. The operator C will also be used later

$$C = \pi - \tilde{\pi}. \quad (4.17)$$

It obeys $C^2 = \mathbf{I}$ and is related to Σ_{12} through the equalities

$$\Sigma_{12} = \frac{1}{2}(1 - C_1 C_2) \text{ and } \mathbf{I} \otimes \mathbf{I} - \Sigma_{12} = \frac{1}{2}(1 + C_1 C_2) \quad (4.18)$$

From the previous operators, one can construct an R-matrix acting on $V \otimes V$ and with spectral parameter λ

$$R_{12}(\lambda) = \Sigma_{12} P_{12} + \Sigma_{12} \sin \lambda + (\mathbf{I} \otimes \mathbf{I} - \Sigma_{12}) P_{12} \cos \lambda \quad (4.19)$$

Several properties of the R-matrix are given in [94], [95]. The most important is the Yang–Baxter equation

$$R_{12}(\lambda_{12}) R_{13}(\lambda_{13}) R_{23}(\lambda_{23}) = R_{23}(\lambda_{23}) R_{13}(\lambda_{13}) R_{12}(\lambda_{12})$$

where $\lambda_{ij} = \lambda_i - \lambda_j$. (4.20)

With a very standard construction, from the R-matrix one constructs the (L sites) transfer matrix (1.30)

$$t_{1\dots L}(\lambda) = \text{strace}_0 R_{01}(\lambda) R_{02}(\lambda) \dots R_{0L}(\lambda) \quad (4.21)$$

by taking the supertrace in the auxiliary space. So far, the calculation has been very general and no special properties of the space V are required. Now, if V has infinite dimension, it is necessary to assume the existence of a trace or supertrace with the cyclic property. If V has finite dimension, the trace always exists. The relation (4.20) implies that the transfer matrices commute for different values of the spectral parameter, thus granting integrability.

Since the R-matrix is regular (namely in $\lambda = 0$ it is a permutation), logarithmic derivatives in $\lambda = 0$ give local operators as in (1.35). The first one can be chosen as XX-Hamiltonian

$$H = t_{1\dots L}(0)^{-1} \frac{dt_{1\dots L}}{d\lambda}(0) = \sum_{j=1}^L H_{j,j+1} \quad (4.22)$$

with $H_{j,j+1} = P_{j,j+1} \Sigma_{j,j+1}$

where periodic boundary conditions have been used, i.e. the site $L + 1$ is identified with the first one.

For example, the original XX model (related to the algebra $gl(2)$) is obtained without gradation with local vector space $V = \mathbb{C}^2$ and 2×2 matrices

$$\pi = E_{1,1}, \quad \tilde{\pi} = \mathbf{I} - \pi = E_{2,2} \quad (4.23)$$

Then the Hamiltonian is the XX model

$$H = \sum_{j=1}^L (E_{12;j} E_{21;j+1} + E_{21;j} E_{12;j+1}) = \sum_{j=1}^L (\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+) = \frac{1}{2} \sum_{j=1}^L (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y)$$

For this reason, (4.22) defines generalized XX models that in [95] were called *universal*. With the same choice (4.23) but using a grading such that the index 1 is bosonic and the index 2 is fermionic, the $gl(1|1)$ XX model has Hamiltonian

$$H = \sum_{j=1}^L (-E_{12;j} E_{21;j+1} + E_{21;j} E_{12;j+1}) = \sum_{j=1}^L (c_j^\dagger c_{j+1} + c_{j+1}^\dagger c_j) \quad (4.24)$$

because the matrices E_{12} and E_{21} are both “fermionic”; they anticommute on different sites so the fermionic realization (4.5) can be used. The index ρ here is not necessary. The relation between the XX model and the Hubbard model is now more clear.

“Gluing” two possibly different universal XX models produces a generalized integrable Hubbard model. The R -matrices of two universal XX models are distinguished by the arrow $R_{12}^\uparrow(\lambda)$ and $R_{12}^\downarrow(\lambda)$. The Hubbard-like R -matrix has two spectral parameters λ_1, λ_2 and is constructed by tensoring on each site an “up” and a “down” copy

$$R_{12}(\lambda_1, \lambda_2) = R_{12}^\uparrow(\lambda_{12}) R_{12}^\downarrow(\lambda_{12}) + \frac{\sin(\lambda_{12})}{\sin(\lambda'_{12})} \tanh(h'_{12}) R_{12}^\uparrow(\lambda'_{12}) C_1^\uparrow R_{12}^\downarrow(\lambda'_{12}) C_1^\downarrow \quad (4.25)$$

where $\lambda_{12} = \lambda_1 - \lambda_2$ and $\lambda'_{12} = \lambda_1 + \lambda_2$. Moreover, $h'_{12} = h(\lambda_1) + h(\lambda_2)$ and the choice of the function $h(\lambda)$ is fixed within the proof of the Yang-Baxter equation. Indeed, when the function $h(\lambda)$ is given by $\sinh(2h) = U \sin(2\lambda)$ for some free parameter U , the R -matrix (4.25) obeys the Yang-Baxter equation:

$$R_{12}(\lambda_1, \lambda_2) R_{13}(\lambda_1, \lambda_3) R_{23}(\lambda_2, \lambda_3) = R_{23}(\lambda_2, \lambda_3) R_{13}(\lambda_1, \lambda_3) R_{12}(\lambda_1, \lambda_2). \quad (4.26)$$

Notice that, this time, the equation is not of difference type. As remarked in [94] the proof relies only on some intermediate properties that are not affected by the choice of the fundamental projectors (4.14). The proof follows the steps of the original proof by Shiroishi [86] for the Hubbard model. The same proof has been used for general $gl(N)$ algebras in [77].

The Hubbard R -matrix is regular but non symmetric. It satisfies unitarity. A commuting family of transfer matrices is obtained by fixing one of the two spectral parameters

$$t_{1\dots L}(\lambda) = \text{str}_0 R_{01}(\lambda, \mu) \dots R_{0L}(\lambda, \mu) \Big|_{\mu=0}. \quad (4.27)$$

Any other choice for μ is possible but, at least in view of obtaining a local Hamiltonian, they do not give new information. The ‘reduced’ R -matrices that enter in the previous equation take a particularly simple factorised form

$$R_{12}(\lambda, 0) = R_{12}^\uparrow(\lambda) R_{12}^\downarrow(\lambda) I_1^{\uparrow\downarrow}(h) \quad (4.28)$$

where

$$I_1^{\uparrow\downarrow}(h) = \mathbf{I} \otimes \mathbf{I} + \tanh\left(\frac{h}{2}\right) C_1^\uparrow C_1^\downarrow \quad (4.29)$$

and one arrives at a Hubbard-like Hamiltonian

$$H = \sum_{j=1}^L H_{j,j+1} = \sum_{j=1}^L \left[\Sigma_{j,j+1}^\uparrow P_{j,j+1}^\uparrow + \Sigma_{j,j+1}^\downarrow P_{j,j+1}^\downarrow + U C_j^\uparrow C_j^\downarrow \right] \quad (4.30)$$

where periodic boundary conditions hold. Clearly, the up and down components are put in interaction only by the potential term $U C_j^\uparrow C_j^\downarrow$. The tensor product of the up and down component is represented in Figure 4.1. Operators “up”, as $R_{12}^\uparrow(\lambda)$, act on the first and third spaces and are the identity on the others while operators “down”, as $R_{12}^\downarrow(\lambda)$, act on the second and fourth. The Hubbard model itself is obtained by two graded $gl(1|1)$ models as in (4.23). Its local (one site) vector space is

$$V = V^\uparrow \otimes V^\downarrow, \quad V^\rho = \mathbb{C}^2 \quad (4.31)$$

The universal Hamiltonian (4.30) has the same structure of the Hubbard model. What can make different the dynamics is the fact that the projectors $\pi, \tilde{\pi}$ seem to introduce several types of particles.

These models were introduced in relation to their symmetries. In [94, 95] it has been shown that the transfer matrix admits as symmetry (super)algebra the direct sum of the symmetry algebras of the XX components

$$\mathcal{S} = \text{End}(W^\uparrow) \oplus \text{End}(\widetilde{W}^\uparrow) \oplus \text{End}(W^\downarrow) \oplus \text{End}(\widetilde{W}^\downarrow) \quad (4.32)$$

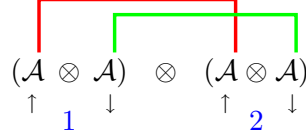


Figure 4.1. This scheme shows the coupling between two universal XX models. The blue indices represent the sites 1 and 2 of the Hubbard model. On each site there is one XX up and one XX down. \mathcal{A} represents the local vector space V or the local algebra $\text{End}(V)$ if vectors or matrices are considered, respectively.

(the up R-matrix commutes with the down generators and vice versa). The generators of the symmetry have the form of the sum of local matrices acting on a single site at a time

$$\mathbb{M} = \mathbb{M}^\uparrow + \mathbb{M}^\downarrow, \quad \mathbb{M}^\uparrow = \sum_{j=1}^L \mathbb{M}_j^\uparrow, \quad \mathbb{M}^\downarrow = \sum_{j=1}^L \mathbb{M}_j^\downarrow \quad (4.33)$$

where

$$\mathbb{M} = \mathbb{M}^\uparrow + \mathbb{M}^\downarrow \quad \text{and} \quad \mathbb{M}^\sigma \in \text{End}(W^\sigma) \oplus \text{End}(\widetilde{W}^\sigma). \quad (4.34)$$

They commute with the monodromy/transfer matrix and with the Hamiltonian.

In this formalism, given that $W^\uparrow = \widetilde{W}^\uparrow = W^\downarrow = \widetilde{W}^\downarrow = \mathbb{C}$, the Hubbard model seems to have just the symmetry algebra

$$gl(1) \oplus gl(1) \oplus gl(1) \oplus gl(1) \quad (4.35)$$

where each term is a single operator

$$\hat{E}_{1,1;\uparrow} = \sum_{j=1}^L E_{1,1;\uparrow j}, \quad \hat{E}_{1,1;\downarrow} = \sum_{j=1}^L E_{1,1;\downarrow j}, \quad \hat{E}_{2,2;\uparrow} = \sum_{j=1}^L E_{2,2;\uparrow j}, \quad \hat{E}_{2,2;\downarrow} = \sum_{j=1}^L E_{2,2;\downarrow j} \quad (4.36)$$

These operators count the number of “particles”. This is more visible after a Jordan-Wigner transformation (4.5): indeed the operator

$$\hat{E}_{2,2;\uparrow} = \sum_{j=1}^L n_{\uparrow j} \quad (4.37)$$

counts how many up fermions are in a given state. Similarly, the operator $\hat{E}_{2,2;\downarrow}$ counts the number of down fermions. From the local (=on site) identity $E_{1,1} + E_{2,2} = \mathbf{I}$, the following sums give the lattice size

$$\hat{E}_{1,1;\uparrow} + \hat{E}_{2,2;\uparrow} = \hat{E}_{1,1;\downarrow} + \hat{E}_{2,2;\downarrow} = L \quad (4.38)$$

so in the symmetry algebra (4.35) there is an amount of redundancy.

It is well known that the Hubbard symmetry algebra is $su(2)$ and becomes $su(2) \times su(2)$ if the number of sites is even. Indeed, the cases where V^σ is two dimensional are special because, in addition to the list of generators contained in (4.32, 4.36), they have new generators given by

$$S_j^\pm = \sigma_{\uparrow j}^\pm \otimes \sigma_{\downarrow j}^\mp, \quad \mathcal{M}_j^\pm = \sigma_{\uparrow j}^\pm \otimes \sigma_{\downarrow j}^\pm. \quad (4.39)$$

To be precise, the first commutes with the Hamiltonian in all cases and promotes the Hubbard symmetry algebra to $su(2)$, where the third generator would be $S_j^3 = \frac{1}{2}(\hat{E}_{2,2;\uparrow j} - \hat{E}_{2,2;\downarrow j})$. The operators \mathcal{M}_j^\pm commutes only if L is even enhancing the symmetry to $su(2) \oplus su(2)$. In that case, the third generator is $\mathcal{M}_j^3 = \frac{1}{2}(\hat{E}_{2,2;\uparrow j} + \hat{E}_{2,2;\downarrow j})$.

Unfortunately, this strongest symmetry doesn’t extend to higher dimensional cases. Some enlargement of the symmetry appears at large coupling in perturbative calculations but it does not survive at higher orders.

$gl(2|2) \oplus gl(2|2)$ Hubbard Hamiltonian

This model implements two identical copies (up and down) of an XX both with

$$\pi = E_{11} + E_{33}, \quad \tilde{\pi} = E_{22} + E_{44} \quad (4.40)$$

and with indices 3, 4 of fermionic nature. Using a graded Jordan-Wigner transformation one arrives at a fermionic form for the Hamiltonian

$$H = \sum_{i=1}^L \left\{ \sum_{\sigma=\uparrow,\downarrow} (c_{\sigma,i}^\dagger c_{\sigma,i+1} + c_{\sigma,i+1}^\dagger c_{\sigma,i}) (c_{\sigma,i}^{\prime\dagger} c_{\sigma,i+1}' + c_{\sigma,i+1}^{\prime\dagger} c_{\sigma,i}' + 1 - n'_{\sigma,i} - n'_{\sigma,i+1}) + U(1 - 2n_{\uparrow,i})(1 - 2n_{\downarrow,i}) \right\} \quad (4.41)$$

where the factor

$$\mathcal{N}'_{\sigma,i,i+1} = (c_{\sigma,i}^{\prime\dagger} c_{\sigma,i+1}' + c_{\sigma,i+1}^{\prime\dagger} c_{\sigma,i}' + 1 - n'_{\sigma,i} - n'_{\sigma,i+1}) \quad (4.42)$$

multiplies an ordinary Hubbard hopping term; only unprimed particles enter into the potential. There are four types of fermionic particles, respectively generated by $c_{\uparrow,i}^\dagger, c_{\downarrow,i}^\dagger, c_{\uparrow,i}^{\prime\dagger}, c_{\downarrow,i}^{\prime\dagger}$ so that they define a 16 dimensional vector space on each site

$$V_{\uparrow,i} \otimes V_{\downarrow,i} \otimes V'_{\uparrow,i} \otimes V'_{\downarrow,i} \quad (4.43)$$

with each $V = \mathbb{C}^2$. The corresponding numbers of particles are conserved.

The factor $\mathcal{N}'_{\sigma,i,i+1}$ works on a 4×4 one-site space; its eigenvalues can be easily obtained and are ± 1 with two-fold multiplicity. This means that it cannot vanish, $\mathcal{N}'_{\sigma,i,i+1} \neq 0$. Moreover, if no primed particles are present, $\mathcal{N}'_{\sigma,i,i+1} = 1, \forall \sigma, i$. The same is true if the lattice is fully filled with primed particles in which case $\mathcal{N}'_{\sigma,i,i+1} = -1$ therefore two of the sectors described by this Hamiltonian are equivalent to the ordinary Hubbard model. A Russian doll structure is appearing: if the projectors are well chosen, a larger model contains the small ones.

If there are primed particles only, the energy vanishes but not the momentum. This actually means that primed particles do not have a dynamics independent of the unprimed. This fact is curious and I am not aware of other cases in which it has been observed. If the potential term is interpreted as a Coulomb repulsion, then unprimed particles only carry electric charge so primed particles are neutral.

The compound objects formed by $c_{\sigma,i}^\dagger c_{\sigma,i}'^\dagger$ are rigid: no other term in the Hamiltonian can destroy them. In this sense, there are four types of carriers, with the same charge but different behaviours: two are the elementary objects $c_{\sigma,i}^\dagger$ in two polarisations $\sigma = \uparrow, \downarrow$, two are the compound objects, in two polarisations.

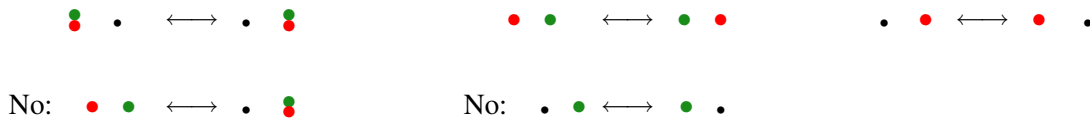


Figure 4.2. The different elementary processes that are described in (4.41); unprimed particles are charged \bullet , primed particles are neutral \circ . The compound object has both the colors. The two lower processes cannot exist, namely the compound object cannot be created or destroyed and the neutral particle alone is static.

The study of the two-particle scattering matrix has been done in [95], with a preliminary account of the Bethe equations. There are general features that emerge. First the vacuum state is chosen as (other choices are possible)

$$\Omega = (e_1^\uparrow \otimes e_1^\downarrow) \otimes (e_1^\uparrow \otimes e_1^\downarrow) \otimes \dots \otimes (e_1^\uparrow \otimes e_1^\downarrow) \quad (4.44)$$

where the index behind the tensor product labels the lattice sites. All other states are considered excitations above it. From the projector π one has to remove the part that projects on the vacuum so the operator $\overset{\circ}{\pi}$ projects on the subspace $\overset{\circ}{W}$

$$\overset{\circ}{\pi} = \pi - E_{1,1}, \quad \overset{\circ}{W} = \overset{\circ}{\pi} V = \overset{\circ}{\pi} W \quad (4.45)$$

Particles are classified by the type, according to the various subspaces $\overset{\circ}{W}^\uparrow, \widetilde{W}^\uparrow, \overset{\circ}{W}^\downarrow, \widetilde{W}^\downarrow$.

Within the universal XX models, all particles satisfy the exclusion principle, namely they cannot appear on the same site. If two particles are both from $\overset{\circ}{W}$ or both from \widetilde{W} , they reflect each other; if they are one from $\overset{\circ}{W}$, one from \widetilde{W} , they traverse each other but still remaining on different sites.

In the universal Hubbard models, the coupling activates a sort of electrostatic interaction felt by particles of opposite “polarisation” only. Indeed, the potential term in (4.30) squares to the identity (4.17) so on one site it has eigenvalues $\pm U$. Which sign occurs is dictated by the membership to $\overset{\circ}{W}$ or \widetilde{W} according to the rule: with $U > 0$, equal type particles (both in $\overset{\circ}{W}$ or in \widetilde{W}) repel each other with an amplitude -1 while different type particles one each from $\overset{\circ}{W}, \widetilde{W}$ attract each other with an amplitude that is just a phase. Observe that the vacuum itself is in the repulsive case so actually the only “visible” effect is the attractive one.

The most important interaction comes when a particle from \widetilde{W}^\uparrow and one from \widetilde{W}^\downarrow meet at a point. This gives rise to the usual transmission and reflection amplitudes of the Hubbard model, $T(p_1, p_2), R(p_1, p_2)$. Notice that they are the same for all particles. The two-particle S-matrix, directly taken from [95], is

$$\begin{aligned} S_{12}(p_1, p_2) &= S_{12}^{X\uparrow}(p_1, p_2) + S_{12}^{X\downarrow}(p_1, p_2) + S_{12}^\uparrow(p_1, p_2) + S_{12}^H(p_1, p_2) \\ S_{12}^{X\rho}(p_1, p_2) &= e^{-ip_1} \overset{\circ}{\pi}^\rho \otimes \widetilde{\pi}^\rho + e^{ip_2} \widetilde{\pi}^\rho \otimes \overset{\circ}{\pi}^\rho - P_{12} \left(\overset{\circ}{\pi}^\rho \otimes \overset{\circ}{\pi}^\rho + \widetilde{\pi}^\rho \otimes \widetilde{\pi}^\rho \right), \quad \rho = \uparrow, \downarrow \\ S_{12}^\uparrow &= \overset{\circ}{\pi}^\uparrow \otimes (\overset{\circ}{\pi}^\downarrow + \widetilde{\pi}^\downarrow) + (\overset{\circ}{\pi}^\downarrow + \widetilde{\pi}^\downarrow) \otimes \overset{\circ}{\pi}^\uparrow + \overset{\circ}{\pi}^\downarrow \otimes \widetilde{\pi}^\uparrow + \widetilde{\pi}^\downarrow \otimes \overset{\circ}{\pi}^\uparrow \\ S_{12}^H(p_1, p_2) &= \left(T(p_1, p_2) \mathbf{I} \otimes \mathbf{I} + R(p_1, p_2) P_{12} \right) \left(\widetilde{\pi}^\uparrow \otimes \widetilde{\pi}^\downarrow + \widetilde{\pi}^\downarrow \otimes \widetilde{\pi}^\uparrow \right) \\ T(p_1, p_2) &= \frac{\sin(p_1) - \sin(p_2)}{\sin(p_1) - \sin(p_2) - 2iU} \\ R(p_1, p_2) &= \frac{2iU}{\sin(p_1) - \sin(p_2) - 2iU} = T(p_1, p_2) - 1 \end{aligned}$$

In summary, the generalizations of the Hubbard model describe new aspects, mainly in relation to the π projector and $\overset{\circ}{W}$ space. They were not present in Hubbard because its space of states is too small. The generalized models can describe many different fermionic particles, all living in the same lattice, some charged and some chargeless. The core of the interactions within \widetilde{W} remains the same as in Hubbard, with the same amplitudes.

The exposition on the generalizations of the Hubbard model stops here.

4.3 A system of two non-linear integral equations for the Hubbard model

Following the methods of Chapter 2, the system of equations for the Hubbard model is introduced. The full derivation is given in the original paper [67]. The main purpose of this work was to study certain super Yang-Mills operators; this has conditioned some choices, as the systematic use of the phase ϕ , which is related to a global magnetic field; of course, the whole construction holds for the Hubbard model itself. Looking at the Lieb-We equations (4.9), I define the function

$$\Phi(x, \xi) = i \ln \frac{i\xi + x}{i\xi - x}, \quad (4.46)$$

with the branch cut of $\ln(z)$ along the real negative z -axis in such a way that $-\pi < \arg z < \pi$. Then, I introduce the gauge transformation which amounts to add the magnetic flux

$$k_j = \hat{k}_j + \phi. \quad (4.47)$$

Using the following counting functions

$$W(k) = L(k - \phi) - \sum_{l=1}^M \Phi \left(u_l - \frac{2t}{U} \sin k, \frac{1}{2} \right), \quad (4.48)$$

$$Z(u) = \sum_{j=1}^L \Phi \left(u - \frac{2t}{U} \sin k_j, \frac{1}{2} \right) - \sum_{m=1}^M \Phi(u - u_m, 1), \quad (4.49)$$

the Lieb-Wu equations take the form of quantisation conditions for the Bethe roots $\{k_j, u_l\}$,

$$W(k_j) = \pi(M + 2I_j^w), \quad (4.50)$$

$$Z(u_l) = \pi(M - L + 1 + 2I_l^z). \quad (4.51)$$

From now on, the treatment focuses on the highest energy state, consisting of the maximum number $M = L/2$ of real roots u_l and of L real roots k_j . For simplicity reasons, it is useful to restrict the calculation to the case $M \in 2\mathbb{N}$ (the remaining case $M \in 2\mathbb{N} + 1$ is a simple modification of this case), which obviously implies $L \in 4\mathbb{N}$.

With the integral definition of the Bessel function $J_0(z)$,

$$J_0(z) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{iz \sin k}, \quad (4.52)$$

and also the following shorthand notations

$$L_W(k) = \text{Im} \ln \left[1 - e^{iW(k+i0)} \right], \quad L_Z(x) = \text{Im} \ln \left[1 + e^{iZ(x+i0)} \right]. \quad (4.53)$$

the first of two nonlinear integral equations for the counting functions is

$$\begin{aligned} Z(u) = & L \int_{-\infty}^{\infty} \frac{dp}{2p} \sin(pu) \frac{J_0\left(\frac{2tp}{U}\right)}{\cosh \frac{p}{2}} + 2 \int_{-\infty}^{\infty} dy G(u - y) \text{Im} \ln \left[1 + e^{iZ(y+i0)} \right] - \\ & - \frac{2t}{U} \int_{-\pi}^{\pi} dk \cos k \frac{1}{\cosh\left(\pi u - \frac{2t\pi}{U} \sin k\right)} \text{Im} \ln \left[1 - e^{iW(k+i0)} \right], \end{aligned} \quad (4.54)$$

where $G(x)$ is the same kernel function that appears in the spin 1/2 XXX chain and in the BDS Bethe Ansatz⁵, as in eq. 2.24 of [96],

$$G(x) = \int_{-\infty}^{\infty} \frac{dp}{2\pi} e^{ipx} \frac{1}{1 + e^{|p|}}. \quad (4.55)$$

The first line of the NLIE for Z (4.54) coincides with the NLIE (eq. 3.15 of [96]) for the counting function of the highest energy state of the BDS model. The second line of (4.54) is the genuine contribution of the Hubbard model. The second nonlinear integral equation is

$$\begin{aligned} W(k) = & L \left[(k - \phi) + \int_{-\infty}^{\infty} \frac{dp}{p} \sin \left(\frac{2tp}{U} \sin k \right) \frac{J_0\left(\frac{2tp}{U}\right)}{1 + e^{|p|}} \right] - \\ & - \int_{-\infty}^{\infty} dx \frac{1}{\cosh\left(\frac{2t\pi}{U} \sin k - \pi x\right)} \text{Im} \ln \left[1 + e^{iZ(x+i0)} \right] - \\ & - \frac{4t}{U} \int_{-\pi}^{\pi} dh G\left(\frac{2t}{U} \sin h - \frac{2t}{U} \sin k\right) \cos h \text{Im} \ln \left[1 - e^{iW(h+i0)} \right]. \end{aligned} \quad (4.56)$$

⁵The Beisert, Dippel, Staudacher model was a deformation of the XXX Bethe equations introduced to describe all loops in the $SU(2)$ sector of SYM, see [96].

The two equations (4.54, 4.56) are coupled by integral terms and are completely equivalent to the Bethe equations for the highest energy state.

The eigenvalues of the Hamiltonian (4.1) on the Bethe states are given by (4.10), that can now be expressed in terms of the counting functions. I use the Bessel function

$$J_1(z) = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \sin k e^{iz \sin k}, \quad (4.57)$$

The highest eigenvalue energy is expressed in terms of the counting functions Z and W as follows

$$\begin{aligned} E &= -2t \left\{ L \int_{-\infty}^{\infty} \frac{dp}{p} \frac{J_0\left(\frac{2tp}{U}\right) J_1\left(\frac{2tp}{U}\right)}{e^{|p|} + 1} + \int_{-\infty}^{\infty} dx \left[\int_{-\infty}^{\infty} \frac{dp}{2\pi} \frac{e^{ipx}}{\cosh \frac{p}{2}} i J_1\left(\frac{2tp}{U}\right) \right] L_Z(x) - \right. \\ &\quad \left. - \frac{2t}{U} \int_{-\pi}^{\pi} \frac{dh}{\pi} L_W(h) \cos h \left[\int_{-\infty}^{\infty} \frac{dp}{i} e^{i \frac{2tp}{U} \sin h} \frac{J_1\left(\frac{2tp}{U}\right)}{e^{|p|} + 1} \right] - \int_{-\pi}^{\pi} \frac{dh}{\pi} L_W(h) \sin h \right\} \\ &\equiv E_L + E_Z + E_{W1} + E_{W2}, \quad \text{and} \quad E_W \equiv E_{W1} + E_{W2}. \end{aligned} \quad (4.58)$$

The first line of (4.58), namely $E_L + E_Z$, coincides formally with the expression of the highest energy of the BDS chain as given in equation (3.24) of [96]. However, in this case Z satisfies a NLIE which is different from that of the BDS model. On the other hand, the second line, i.e. $E_W = E_{W1} + E_{W2}$, is a completely new contribution.

This system of equations can be extended to include all excitations. Indeed, one has to include appropriate sources for the real holes and for all the complex roots that can appear, precisely as in (3.47). The main goal of the papers [96, 67] was, however, to use the nonlinear integral equations for a careful investigation of several limits: large volume (large L expansion, namely a thermodynamic limit), strong ($U \rightarrow +\infty$) and weak coupling ($U \rightarrow 0$) and possibly to study the effect of interchanging the order of the limits. At the beginning of this work (2005-2006) the belief was that the Hubbard model could represent anomalous dimensions of the $\mathcal{N} = 4$ super Yang-Mills theory. Within this correspondence between Hubbard and super Yang-Mills, the study of the large volume limit corresponds to study very long super Yang-Mills operators. In Figure 4.3, the energy (4.58) is plotted as function of the coupling constant, for a lattice of 12 sites.

4.4 Discussion

I have presented two different works on the subject of the Hubbard model in relation to the $\mathcal{N} = 4$ super Yang-Mills theory. Both of them have been developed in the years 2005-2007 and were amongst the first attempts to use integrability techniques in the gauge theory.

The integrable generalizations of the Hubbard model were introduced in [94]. In [95] I have started to work on the derivation of the Bethe equations. The scattering matrix is fully presented in that article. The full set of Bethe equations has been obtained more recently by colleagues of mine [98].

The work on the nonlinear integral equations for the Hubbard model in [67] was actually the continuation of a work presented in [96] on the XXX model with excitations of type hole, on the BDS Bethe ansatz [82] and on the $SO(6)$ spin chain. I treated these models in the frame of the integrability within the $\mathcal{N} = 4$ super Yang-Mills theory. Today we know that these models are at best approximations of the correct Bethe equations [81]. In spite of this, it was important to start working with the methods presented here. The work of [67] has shown to the community of SYM that the methods of nonlinear integral equations are effective in treating certain questions starting from Bethe equations. For this reason, my co-authors are still active in the field. They have treated a number of new cases, including models with non-compact symmetry groups, large number of holes, etc. [99].

After these publications, my research activities have taken a new direction, that will be presented in the next chapters.

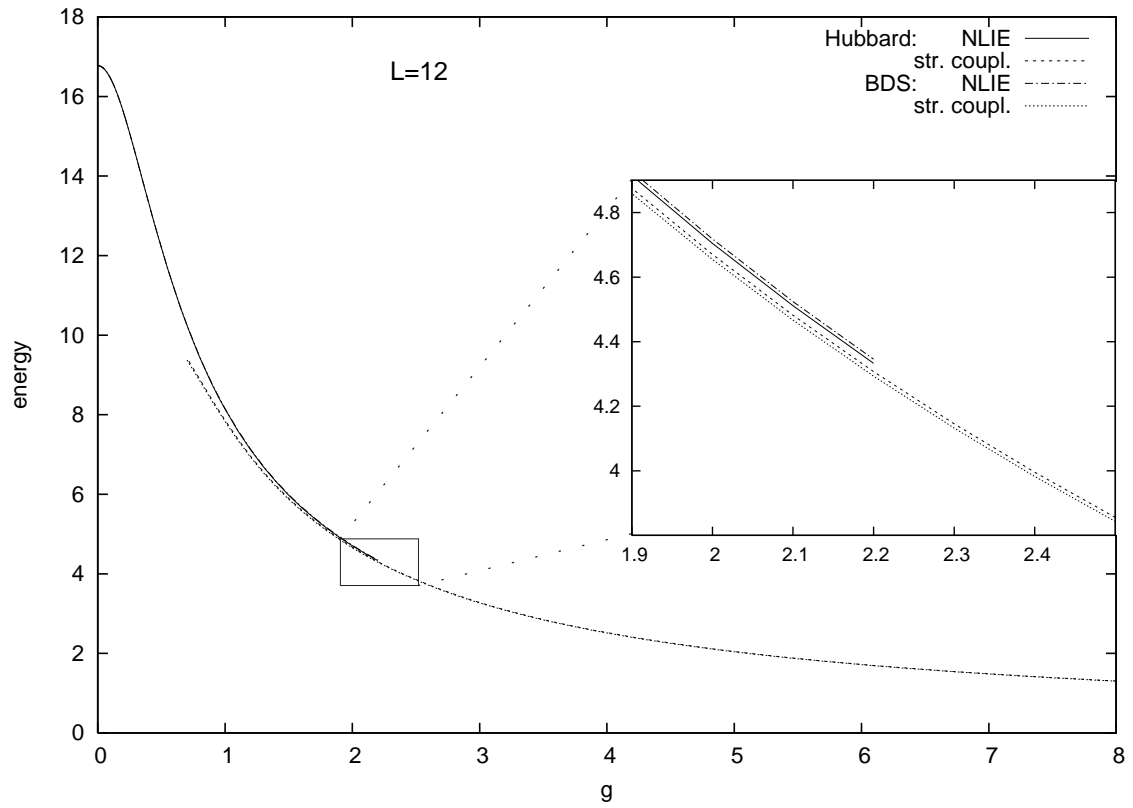


Figure 4.3. The behaviour of the energies for Hubbard and BDS model from small to strong coupling is plotted here for a lattice of 12 sites. The left branches of the curves are obtained by solving numerically the NLIE while the right branches are plotted using the the strong coupling expansion from the NLIE. In the small picture there is a zoom of the region where the branches overlap. The approximated match is due to numerical errors in the left curve.

Bibliography: Integrability

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Part II

Biophysics: quantitative methods for biology

Motivations

The application of quantitative methods to biology is presently the object of a large amount of theoretical studies. Theoretical study and modeling of biological phenomena are not a substitute to biological *in vivo* investigation. Instead, they are a very “economical” way to formulate quantitative relations between relevant quantities and to make predictions with them.

Nowadays, modeling biological phenomena corresponds to the approach that has been adopted innumerable times in other domains of science, especially physics. Weren’t the three Kepler’s laws a model? Of course they were. Kepler was not aware of more fundamental and general laws to use (namely Newtonian mechanics and gravity), he just formulated a quantitative description of his observations. The Bohr-Sommerfield quantization of adiabatic invariants was a model for old quantum theory. In these examples the model preceded the theory and somehow helped formulating it. Of course, the model can follow the theory and somehow simplify it, as the Ising model for magnetism simplifies a full quantum mechanical approach to the problem. The power of computers makes it possible to develop theoretical tools and models to elaborate and speculate on the vast amount of data accumulated on the genome and on the proteome.

Strongly motivated by this, in collaboration with Dr. F. Musso of the University of Burgos, in 2006 I introduced a model of evolution based on a population of “Turing machines”. Each machine is actually defined by a finite number of “states” that form its own code or genome. This code undergoes stochastic evolution with certain rates that implement different aspects of genome mutation. Then, a performance based selection process creates a new generation of machines with increased performance. The process is repeated for a large number of generations. The goal of this model is to explore features of the Darwinian evolution with a full control of the parameters that participate to it. Indeed, *in silico* evolution and mathematical modeling are ideal environments to test evolutive hypotheses that are otherwise difficult to test in the real biological environment.

In a similar spirit, in 2007 I co-founded the Gemini team in Annecy, with C. Lesieur, biologist, and other collaborators from the mathematical-physical background of the “Federation de recherche Modelisation, Simulation, Interactions Fondamentales”. The team agreed to work on questions of assembly in oligomeric proteins⁶. The team biologist had already approached the subject with standard experimental tools but needed to use theoretical methods describe the problem in general terms through the analysis of a larger number of cases.

A mathematician, L. Vuillon, is part of the Gemini team. This is a signal that the project on the oligomeric proteins has a sufficiently high degree of “synthesis”, in the Greek sense, to be effective in biology and to require a theoretical development as a complex system.

The approach that we carry on is inductive, based on the systematic analysis of structure data of oligomeric proteins. I will present it later. The research is revealing features related to the process of the interface formation and to the process of the assembly of different chains.

The inductive reasoning, which goes from specific observations to broader generalizations and theories, is not always applied in mathematical and theoretical physics. Indeed, it is typical of the periods when a paradigm, or theory, is missing but a scenario is emerging from observations, that forces to move toward a more accurate and complete understanding. Deductive reasoning is common when the paradigm

⁶Oligomeric proteins are those whose native state, or functional state, is the aggregate of two or more polypeptidic chains.

is established and can be applied to predict a variety of phenomena. Modelization is intermediate because the construction of the model often comes from empirical knowledge but the model allows one to deduce further effects.

I hope the next two chapters on biophysics will suggest why a theoretical physicist, like me, is engaging in research on evolution and proteome, and how he can help in the inductive reasoning towards a paradigm.

Chapter 5

Modelling Darwinian evolution

Darwinian evolution is the today paradigm that unifies paleontological records with modern biology. It creates a bridge between the microscopic view (genome, proteome) and the macroscopic features of the living organisms (phenotype). The phenotypic, or macroscopic, mechanism of Darwinian evolution is natural selection namely a differential scrutiny of the phenotypes by environment. The microscopic mechanism is genome mutations. In neodarwinism, it is very important to appreciate the fact that even if the genome is a physical memory that is transmitted from the parent(s) to the offspring, the phenotype of a single organism is not inherited: if a person loses a leg, its children will still have both of their legs. Notice that the physical memory or genome is also under control of the selection so it is correct to say that the genome is part of the phenotype. The opposite is false: the phenotype is not contained in the genome, otherwise it would be automatic to inherit acquired characters, as in Lamarckism.

The basic functioning of the genome¹ is to record long sequences of four letters that later on can be mapped into amino acid sequences by a known mapping that biologists call “the genetic code”. This means that the biological function of proteins, intrinsically three-dimensional and based on physico-chemical properties of atomic aggregates, can be described by a discrete and finite amount of information. It’s unavoidable to imagine that amount of information as being an algorithm that, executed with given rules, realizes some tasks. This analogy between genome and algorithm pervades the whole domain of the artificial life [2] namely the tentative of realizing *in silico* organisms that exploit the main features of living organisms².

The need of modeling Darwinian evolution, or else the need of creating an artificial life, comes from several directions all related to the difficulty to make quantitative experimental studies: we cannot rewind the Earth history to study past organisms “alive”, the fossil record is incomplete, *in vitro* evolution experiments are long and expensive and only few of them have successfully been done. Moreover, the biggest difficulty is to keep apart the different causes that produce the observed evolutionary dynamics. In this scenario, *in silico* evolution can help precisely where observation biology fails: *in silico* experiments can be done on today’s calculus grids, the control on the parameters is complete and the full record of the evolution is available. I cannot avoid a comparison with cosmology: we know a single universe, we cannot rewind its history and observational data on far objects (in remote time and in space) are few. The difference is that artificial cosmological experiments are just impossible while artificial evolution experiments are possible and will slowly be realized. In this sense, biological evolution is much more affordable than cosmology. From Maynard Smith, one reads: “...we badly need a comparative biology. So far, we have been able to study only one evolving system and we cannot wait for interstellar flight to provide us with a second. If we want to discover generalizations about evolving systems, we will have to look at artificial ones.” Modeling evolution has definitely not the goal to replace observatory or experimental biology but has the goal to help finding “universal” features in the evolutionary dynamics

¹Here a possible distinction between genome and DNA is not needed

²More or less, one can summarize them in: existence of a separation interior/exterior, existence of a metabolism, response to external stimuli, self-identical reproduction.

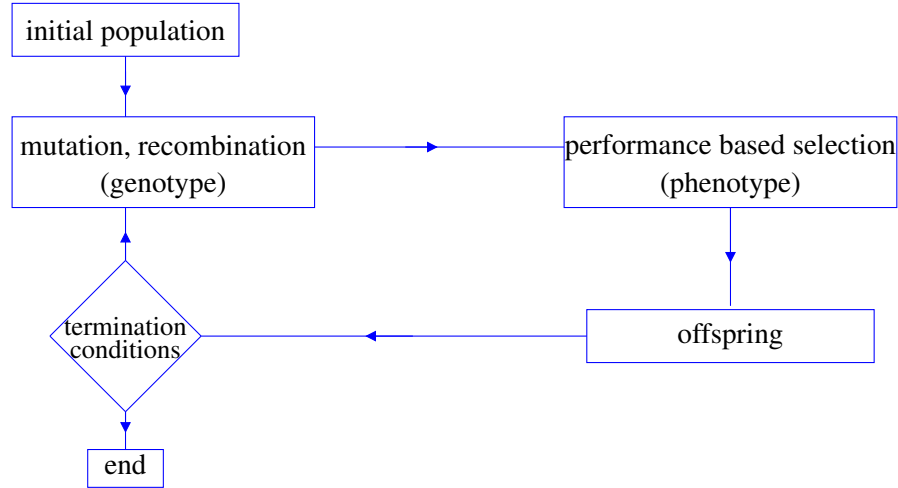


Figure 5.1. Basic flow of evolutionary computations or artificial life cycle. Notice the distinction of genotype and phenotype.

and in the mechanisms of mutation, selection. After all, universality is the way critical phenomena are studied in statistical mechanics: specific details do not participate in determining universal features. This point has been particularly stressed in my recent article [1].

The existence of a small genome within a much larger phenotype and the basic functioning by the genetic code are strategic for modelization purposes because they allow to investigate at least some of the features of evolution without paying too much attention to the whole organism and its proteome but just focusing on algorithm features.

5.1 The model

The idea is to have a population of algorithms that evolve with generations. At each generation, each algorithm undergoes mutation (possibly in several flavours). The algorithm is then executed, which corresponds to the life of the organism. The output represents the phenotype and the interaction with the environment, therefore selection acts on it. The selection, precisely as in the biological case, evaluates differentially two or more phenotypes retaining the best fitted for reproduction. This creates an artificial life cycle, as in Figure 5.1, that can be repeated a large number of times, to study the evolution of the population features.

In my Turing machines model, the algorithms are precisely the Turing machines. This choice was mainly motivated by the generality attained by the Turing machines language, in spite of a very simple set of basic instructions. This aspect is extremely important as it allows to do some theoretical investigation of the model. Many other formalizations of algorithms have actually been adopted in evolutionary computation [2].

Turing machines are abstract symbol-manipulating devices that implement a “one-point” discrete evolution law. Given a finite alphabet or list of symbols \mathcal{A} and given the total number of internal “states” N_t , one defines a Turing machine by giving the evolution law Q

$$(r, s) \xrightarrow{Q} (r', d', s'), \quad r, r' \in \mathcal{A}, \quad d' \in \{R, L\}, \quad s, s' \in \{1, 2, \dots, N_t\} \quad (5.1)$$

It is the set of actions that the machine performs, determined by the value read on the tape $r = r(t)$, at a position $x_0(t)$, and by the internal state of the machine $s = s(t)$. These variables depend on the execution time, so $r' = r(t+1)$ and so on. Notice that the mapping Q does not depend on the old displacement right/left $d(t)$ but it produces the new displacement $d' = d(t+1)$. The mapping Q is the

state read	1	2	3
0	1 – Right – 2	0 – Left – 3	_ – _ – _
1	1 – Right – 1	1 – Right – 2	0 – _ – Halt

Table 5.1. Table of states of a Turing machine that performs the sum of two positive numbers represented by “sticks”: ... 0 1 1 1 0 0 represents the number three and so on. Missing entries are irrelevant and can be fixed arbitrarily. Here and in the following, the states of the machine are written in bold character, to ease the reading.

core of the Turing machine and can be represented by the triplets “write,displace,call” (w, d, c) acting on a tape, as in table 5.1 and in figure 5.2:

1. **write:** it writes a new symbol at position $x_0(t)$,
2. **displace:** it moves right R or left by one cell L,
3. **call:** it changes its internal state.

An initial configuration is given by assigning the function $T(x, 0) \in \mathcal{A}, \forall x \in \mathbb{Z}$. Recursively, a new configuration $T(x, t + 1) \in \mathcal{A}, \forall x \in \mathbb{Z}$ is computed from $T(x, t)$ with the mapping Q in such a way that only a single mutated position $x_0(t)$ can exist at each time

$$T(x, t + 1) = T(x, t) \quad \forall x \neq x_0(t)$$

$$T(x_0(t), t + 1) \text{ could be } \neq T(x_0(t), t)$$

and such that $x_0(t + 1) = x_0(t) \pm 1$. Here I will use the binary set of symbols $\mathcal{A} = \{0, 1\}$. This choice is mainly dictated by the simplicity of coding it offers. Representing $T(x, t) \forall x$ by a tape of cells at position $x \in \mathbb{Z}$, one has the familiar representation of figure 5.2.

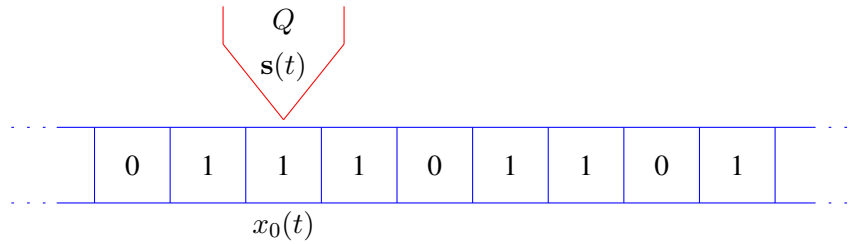


Figure 5.2. Graphical representation of a Turing machine at time t , in the internal state $s(t)$, located on the $x_0(t)$ cell of an infinite tape.

Considering that the general characterization of Turing machines is not needed here, for computational reasons the tape is taken of finite length usually fixed to $L = 300$ boxes. In some simulations the tape has been “periodized”, by identifying the last cell+1 with the first one. Periodic boundary conditions were also used in lattice models. Moreover, as it is extremely easy to generate machines that run forever, the maximum of 4000 temporal steps is imposed. When a machine reaches it, it is stopped and its tape is taken without further modification.

The simulations start with a population of $n_{pop} = 300$ Turing machines each with just one state of the following form

	1
0	0 – R – Halt
1	1 – R – Halt

and go on for $ngen = 50000$ generations or more. At each generation every TM undergoes the following three processes, in the order:

1. (insertion) states-increase,
2. (point) mutation,
3. selection and reproduction.

In the states-increase process, with a probability p_i , the TM passes from N_t to $N_t + 1$ states by the addition of the further state

	$N_t + 1$
0	0 – R – Halt
1	1 – R – Halt

This state will be initially non-coding since it cannot be called by any other state. Indeed, the Turing machine cannot call a state that does not exist. The only way this state can be activated is if a mutation in an already coding state changes the state call to $N_t + 1$. Notice that, when called, this particular state does not affect the tape but halts the machine. Consequently the activation of this state is mainly harmful or neutral and it can be advantageous only in exceptional cases therefore the TM can benefit from the added states only if they are mutated before their activation. This form of mutation vaguely resembles DNA insertion.

During point mutation, all the entries of each state of the TM can be randomly changed with a probability p_m . The new entry is randomly chosen among all corresponding permitted values excluded the original one. The permitted values are:

- 0 or 1 for the “write” entries;
- Right, Left for the “move” entries;
- The **Halt** state or an integer from 1 to the number of states N_t of the machine for the “call” entries.

This mechanism of mutation is reminiscent of the biological point mutation. Notice that the states-increase process is actually a form of mutation. Here it has been chosen to keep the two mutations separate in order to differentiate their roles. Other biological mechanisms like traslocation, inversion, deletion, etc. are not implemented.

In the selection and reproduction phase a new population is created from the actual one (old population). The number of offspring of a TM is determined by its “performance” and, to a minor extent, by chance. The performance³ of a TM is a function that measures how well the output tape of the machine reproduces a given “goal” tape starting from a prescribed input tape. It is computed in the following way. The performance is initially set to zero. Then the output tape and the goal tape are compared cell by cell. The performance is increased by one for any 1 on the output tape that has a matching 1 on the goal tape and it is decreased by 3 for any 1 on the output tape that matches a 0 on the goal tape.

As a selection process, I use what in the field of evolutionary algorithms is known as “tournament selection of size 2 without replacement”. In it, two TMs are randomly extracted from the old population and let run on the input tape. At the end, a performance value is assigned to each machine on the basis of its output tape. The performance values are compared and the machine which scores higher creates two copies of itself in the new population, while the other is eliminated. This reproduction is fully asexual. If the performance values are equal, each TM creates a copy of itself in the new population. The two TMs that were chosen for the tournament are eliminated from the old population and the process restarts until the exhaustion of the old population.

³The word “performance” is preferred to “fitness” as this last one indicates two different concepts in biology and in the field of algorithms. The word “fitness” will be used in the biological sense.

The goal tapes are chosen according to the criterion of providing two difficult and qualitatively different tasks for a TM. The distribution of the “1” on the goal tape has to be extremely non-regular since a periodic distribution would provide a very easy task for a TM.

In the various simulations several goal tapes have been used. The tape “primes” has “1” on the cell positions corresponding to prime numbers, with 1 included for convenience, and zeros elsewhere:

```
1110101000.1010001010.0010000010.1000001000.1010001000.0010000010.1000001000.1010000010.
0010000010.0000001000.1010001010.0010000000.0000001000.1000001010.0000000010.1000001000.
0010001000.0010000010.1000000000.1010001010.0000000000.1000000000.0010001010.0010000010.
1000000000.1000001000.0010000010.1000001000.1010000000.0010000000.
```

In the previous expression I inserted a dot every ten cells to facilitate the reading. The second goal tape π is given by the binary expression of the decimal part of π , namely $(\pi - 3)_{\text{bin}}$:

```
0010010000.1111110110.1010100010.0010000101.1010001100.0010001101.0011000100.1100011001.
1000101000.1011100000.0011011100.0001110011.0100010010.1001000000.1001001110.0000100010.
0010100110.0111110011.0001110100.0000001000.0010111011.1110101001.1000111011.0001001110.
0110110010.0010010100.0101001010.0000100001.1110011000.1110001101.
```

Notice that while for prime numbers the “1” become progressively rarer so that the task becomes progressively more difficult, in the case of the digits of π they are more or less equally distributed. Another difference is that prime numbers are always odd (with the exception of 2) therefore in the goal tape two “1” are separated by at least one “0”. On the contrary, the digits of π can form clusters of “1” of arbitrary length; this feature is actually visible only in very long tapes of thousands of cells or more and is not important here.

According to the definition, the maximal possible value for the performance is 63 for the prime numbers and 125 for the digits of π .

In [3], the objective was introduced of gathering “1” on the left side of the output tape, simulating the process of resources accumulation. The actual definition of the score is involved so it will not be written here.

5.2 Results

In [4] the dependence of the performance by the external parameters p_m, p_i was studied with both the output tapes indicated. The two series of simulations show very similar features. The most evident effect is that having a large amount of non-coding states speeds up evolution and allows to reach larger values of the population performance, as in Figure 5.3. It is important to remember that when new states are added by the states-increase process, they are and remain non-coding until activation by point mutation. Of course, the model has a bias toward the growth of the number of states, because no deletion is introduced and no cost for large genomes is used. This bias is on the total number of states, not on the actual number of coding triplets. The latter is not biased, it can both increase and decrease. This bias

1. **implies** that the total number of states N_t cannot decrease but
2. **does not imply** that the performance grows faster if N_t is large. For this reason, there is no need to add deletion or metabolic costs for large genomes.

The total number of triplets is approximately

$$N_t \approx 2(1 + n_{\text{gen}} \cdot p_i) \quad (5.2)$$

If N_c is the number of coding triplets, the ratio N_c/N_t has been measured and it is of the order of few percent, often less, so approximately $N_{\text{nc}} = N_t - N_c \approx N_t$ is the number of non-coding triplets. The

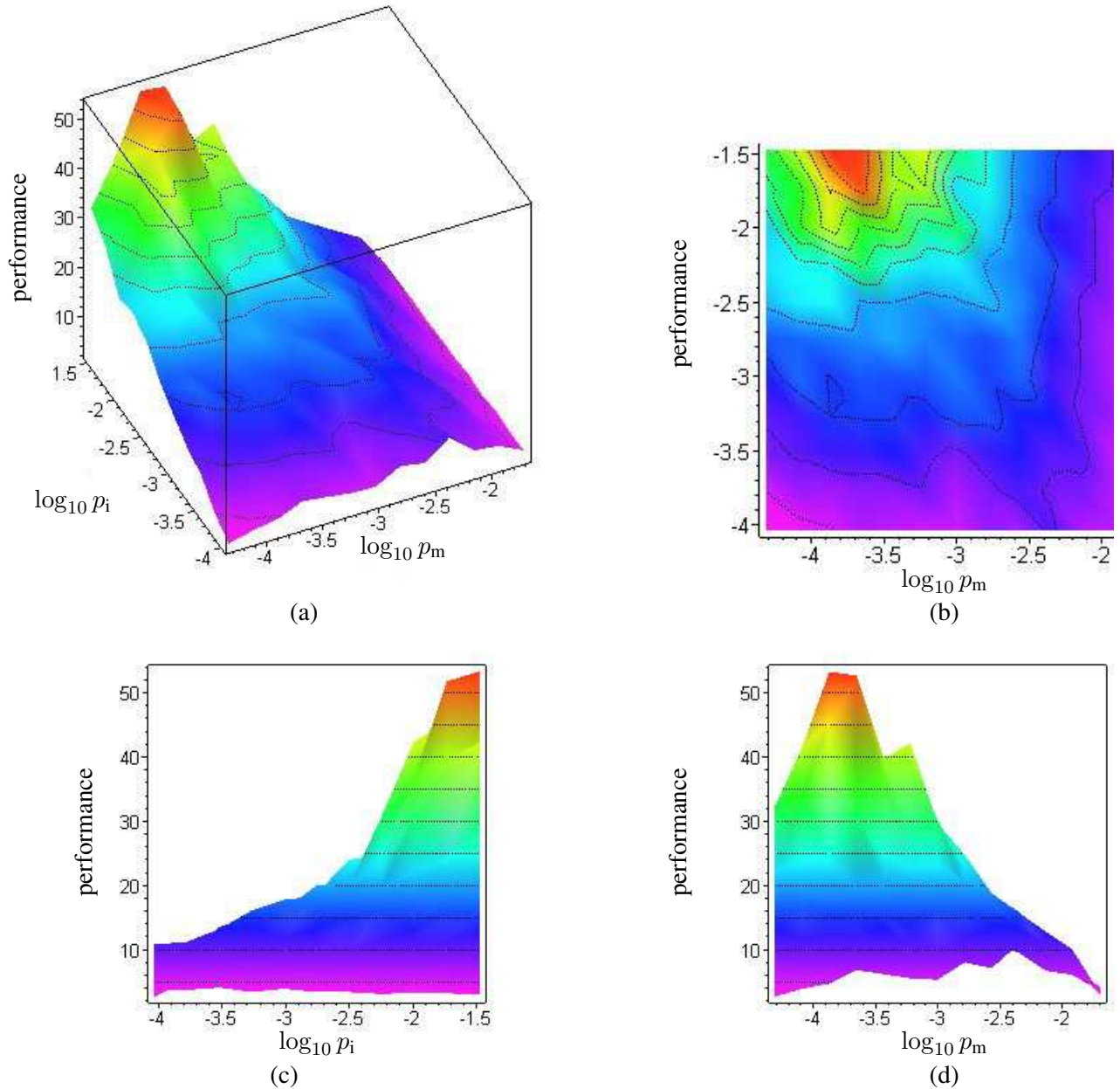


Figure 5.3. For the goal π , in (a) it is shown the 3D plot of the best performance value in the population, averaged on the ten different seeds of the simulation, as function of the states-increase rate p_i and of the mutation rate p_m . The three orthogonal projections of (a) are also shown.

ratio N_c/N_t is observed to decrease with the growth of the performance. This enhances the effect of “reservoir” of the non-coding triplets: simulations show that the performance grows faster if N_{nc} is large, Figure 5.3 (a) and (c), Figure 5.4. This means that the non-coding triplets are used to explore new strategies. While the phenomenon in itself is not totally unexpected, its amplitude and persistence surprises. Several simulations, in part not yet published, seem to indicate that the phenomenon continues at higher p_i with a ratio $N_c/N_t < 0.5$ namely with an enormous excess of non-coding versus coding triplets. It is important to stress that N_t is positively selected, namely it is larger than the value attained in the absence of selection (random evolution). Also, N_{nc} is larger than in the random choice case. As the bias is present with and without selection, the effect on N_t is not produced by the bias. It is a real effect, indirectly produced by selection. It is indirect because the algorithms of selection do not act on N_t .

Besides numerical investigations, the model allows one to perform some analytical evaluations. The spirit of the papers [5, 1] has been precisely to develop a mathematical description of the mutation-selection dynamics and complete it with numerical data. The mutation-selection dynamics is the set of rules that are used by the Turing machines evolving population during simulations. They can be treated mathematically, thus showing the presence of an error threshold. This is a value of the mutation probability p_m^* such that if $p_m > p_m^*$ the highest performance class degrades faster than it is generated; said otherwise, the occupation number of the highest performance class reduces to zero in such a way that the population performance decreases. Degradation is due to harmful mutations, that are very frequent events. Generation is due to rare good mutations and mainly to the selection mechanism, that favours the replication of high performance individuals. Moreover, the population evolves toward the error threshold; this means that, granted a sufficiently large number of generations, the population will occupy all the performance classes up to the error threshold.

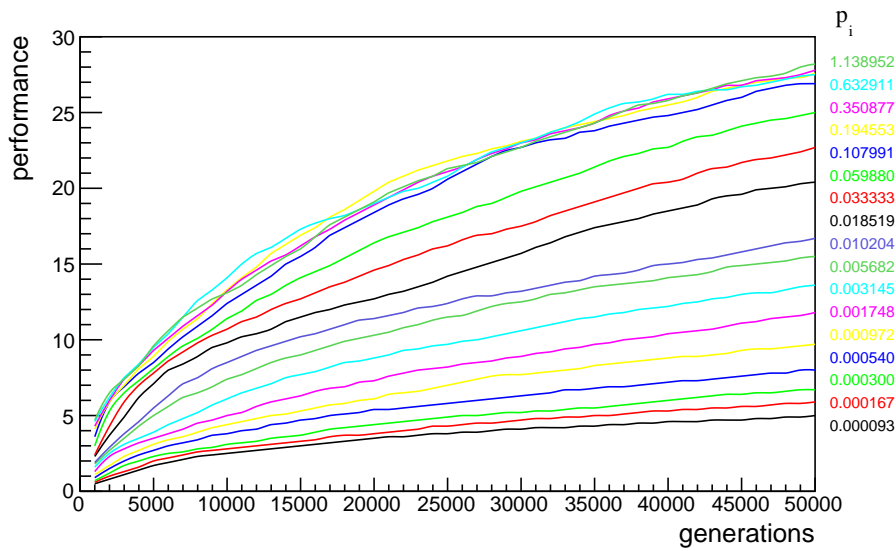


Figure 5.4. The evolution of the performance with the generations, at various values of the state-increase rate. Notice the overlap of the four highest lines, possibly related to the presence of a plateau in the plot of the performance versus p_i . This interpretation is reasonable but still uncertain and difficult to prove because of computational time.

The error threshold evaluated in [1] is

$$p_m^* = 1 - 2^{-\frac{1}{3N_c^*}} \quad (5.3)$$

Both of these effects are shown in Figure 5.5. The black thick line represents the relation between the critical number of coding triplets N_c^* and the error threshold p_m^* . It is never crossed by the averaged population data. Clearly, the error threshold equation expresses quite a general feature of the systems evolving by random mutation and performance based selection: the effect of random mutations is to put an upper bound to the size of the genome. The only way to escape this fate is to reduce the effect of mutations by using reparation mechanisms, optimization, small coding part in a large non-coding genome...

Other effects studied with the Turing machine model include the extinction time of the machines and the evolutive effect of punctuated equilibria.

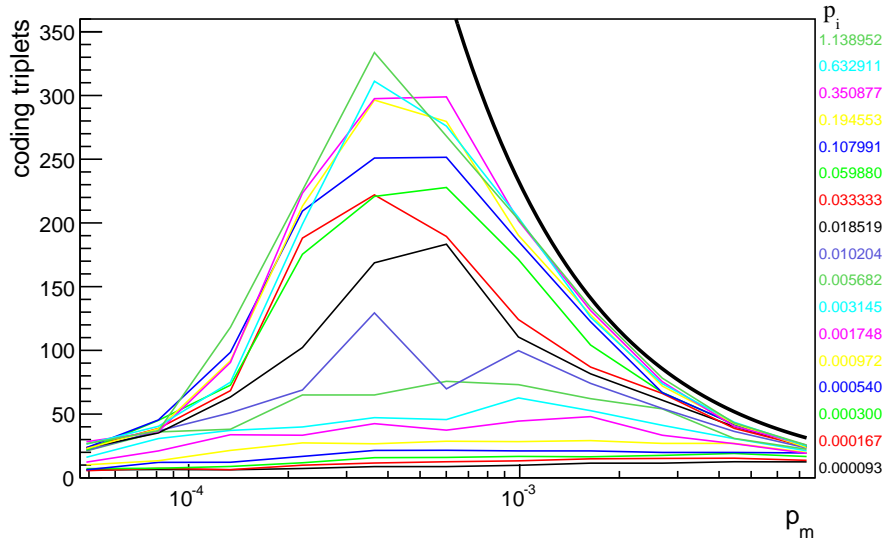


Figure 5.5. The average number of coding triplets $\langle N_c \rangle$ at the end of simulation ($n_{gen} = 50000$) is shown as a function of p_m , for all the values p_i . The value N_c is taken for the best performing machine in the population and is averaged on the seeds. The black thick line on the right represents the critical number of coding triplets N_c^* , as function of p_m^* , extracted from (5.3).

5.3 Discussion

The Turing machines model has been introduced by myself and F. Musso in 2007. From the first paper [4] on, the model has been used for mathematical evaluations and several numerical investigations [5, 1, 3]. One of the next challenges will be to introduce recombination and study the evolution and maintenance of sexual reproduction, a very general reproductive form in nature that is still theoretically poorly understood. Work in this direction has been carried on during the internship of my master student [3].

At the very beginning of this Turing machines program, it wasn't clear to me if the model was just a personal exercise or if it could be of some use. The positive answer came later, by comparing with other evolutionary models and also by appreciating that the TM model could be developed in several directions, for example the one already cited of sexual reproduction.

There are not many other evolutionary models designed to study Darwinian evolution, the most famous one being Avida [6] with its ancestor Tierra [7]. They both are elegant and complete platforms that create an in silico life. Organisms are programs that live on computer grids and compete for resources: CPU time and memory. The simplicity is not the feature of these models, neither is the parsimony in terms of computer resources.

A model that is much closer to TM has been developed by some members of the Institute of complex systems in Lyon [8]. Their model "Aevol" has both a genome and a proteome therefore it implements the transcription/translation mechanism.

In common, all these models have the idea that the genome is an algorithm that is created by random mutations and is selected on the basis of its performance, as in Figure 5.1, measured by the ability of realizing some task: self-replication in the Avida platform, evaluation of some complex mathematical function in Aevol and Turing. Of course, they all have an incomparably lesser degree of complexity than living organisms. More importantly, they do not try to describe the DNA by some "close" description or the protein functions by some catalytic process. Is this a real difficulty? Probably it would be of interest to describe a "realistic" genome, with four bases, the genetic code, the mRNA and amino acid sequences.

One could try to simulate the evolution of very basic enzymatic functions in bacteria. To do that, one should find the “functional site” of a protein from its amino acid sequence, with one of the prediction tools that are known to work. In perspective, this project offers an interesting development but, so far, it has not been realized. Instead, all the cited models claim that a certain algorithm can simulate a genome; they claim that a mathematical function can represent the phenotype and work with these simplifying hypotheses.

Given that, the problem of knowing if realistic results can emerge from non-realistic models is conceptually extremely important. I think the answer that all these authors implicitly assume is very deep and smart: no matter the details of the model, results are universal if universal hypotheses have been formulated. “Universal” is employed in the sense of Kadanoff and Wilson, as it is used in statistical physics and in the renormalization group. Therefore, having different models is important because the comparison of their features and predictions leads to understand which are the universal features of evolution.

Chapter 6

Protein assembly

A large number of proteins become biologically functional only after association of a number of amino acid chains. The ensuing structures are called oligomers. In addition to folding, the oligomers need to assemble, which takes place through the formation of interface areas that are mutually interacting. From [9], one learns that 20% of the proteins in *Escherichia coli* are monomeric, the rest oligomeric/polymeric, with a clear preference for dimers (38%) and tetramers (21%). Amongst oligomers, the large majority is homooligomeric. Few are true polymers. In general, polymers differ from oligomers by their variable stoichiometric number, that can take values of hundred to millions of subunits. In the Protein Data Bank (PDB), 20% only of the recorded proteins are oligomers. It has been noticed, however, that the Protein Data Bank (PDB) over-represents small monomers, because of the difficulties in protein crystallization, thus the value of 20% is underestimated. Given all these data, the importance of investigations of oligomeric proteins is apparent.

Folding and assembly are two processes that occur in oligomeric proteins after ribosomal synthesis. It is believed that in most cases at least a partial folding is required before the assembly can start. The reason for this is that assembly requires the encounter of at least two parts that are in solution in the cell; this process is diffusion limited and can be quite lengthy. In spite of this, it is known that sometimes a “fly-casting” mechanism takes place in which assembly comes very early and the several subunits fold together only after assembly. Thus, the two processes cannot be considered as separated and independent from each other. Moreover, in the first case, it is reasonable to expect at least a partial rearrangement of the structure after assembly.

Even if the microscopic description of folding and assembly undergoes the principles of molecular dynamics-molecular mechanics approaches, it would be of great value to obtain a more macroscopic understanding. Some of the relevant questions are now indicated. What does differentiate two amino acid sequences, one incapable of association, the other capable? Namely, given an unknown sequence, can one predict if it will give rise to a monomer or to an oligomer? Is it possible to predict, from the sequence, which amino acids will constitute the interface? What will be the interface three-dimensional form?

These questions are not so different from those of protein folding. For example, given the sequence, it is possible to do secondary structure predictions because it has been shown that certain groups of few amino acids have particular propensities to one or other possible secondary structure. For example, this has lead to formulate the Chou-Fasman rule. These predictions, however, are not free of errors.

In a similar fashion, it is reasonable to imagine that groups of amino acids or perhaps certain secondary elements have a propensity to form or not interfaces. Or else, there is a propensity for interfaces of a specific geometric form. Are there propensities for a preferred association mechanism? Notice that examples are known where sequences with 90% of identity follow different association patterns. This means that few key amino acids can actually decide the association mechanisms and, why not, the folding itself. These and other questions motivate the present studies on oligomeric proteins.

Important is to focus on the interfaces. In an oligomeric protein the interface has a high degree of

specificity and is very stable. Indeed, the mutual recognition of the two sides of the interface is extremely accurate. Early it was recognised that this happens if the interface is made of many weak “contacts” [10], namely hydrogen bonds, and if the geometric and chemical arrangements of atoms on the two parts are complementary [11]. Indeed, strong contacts, as in a ionic bond, would be able to attract and fix several different molecules so they would be non specific. Absence of complementarity would increase the interatomic distance thus reducing the strength of the contacts and possibly creating space for spurious molecules of water.

The project that I will detail in the next sections focuses on the interfaces of trimeric and higher stoichiometry proteins. Using experimental approaches, it has been observed that few residues, located on the interface of a protein oligomer, are crucial for its assembly. Some of them control the formation of interfaces (association steps) while others control the stability of the oligomer (maintenance of the associated state) [13]. These key residues are not necessarily conserved among proteins of identical function or even of similar fold [14]. This could mean that the few residues dedicated to protein assembly would have to be identified experimentally, for each particular case. Alternatively, a theoretical approach could reveal which features characterize interfaces, by a systematic investigation of the known three dimensional structures of protein interfaces. There are about 4000 cases deposited on the PDB data bank, from the trimeric to the dodecameric stoichiometry. The aim is to identify key residues involved in the different steps of the protein assembly and possibly to derive some of the basic principles that manage protein assembly.

To this purpose, I have created a series of programs (Gemini) that sort out the protein interfaces and describe them as interaction networks (graphs). The interface structure is thus efficiently coded into graphs that allow to identify (or at least propose) the chemical links responsible for the interface’s formation. At present, 3000 cases have been screened. The programs have been successfully tested on known protein interfaces.

6.1 Gemini

It is a series of programs and database utilities that have been created under the common name of Gemini to investigate properties of the interfaces of oligomers: presently, the most important are GeminiDistances, GeminiRegions, GeminiGraph and GeminiData [15].

These programs come from the need to make systematic the analysis of oligomeric interfaces in three-dimensional protein structures. The main criterion followed has been to propose a framework of the amino acid interactions involved in an interface so their role in providing the interface its specificity and in regulating the mechanism of assembly can be addressed, for example by comparing protein interfaces of similar geometry. The objective is to find all pairs of atoms (one atom per chain) located at distances small enough for intermolecular interaction, and to reduce this set of interaction pairs to a minimum: the smallest set that still describes the protein interface.

6.1.1 GeminiDistances

This program has the main goal to recognize the interface between two adjacent chains M and M+1 in an oligomeric protein from its 3D structure.

A first screening is done on the backbone α carbons of adjacent chains: all pairs of amino acids (one per chain), whose $C\alpha$ are separated by a distance lower than a given cut-off, fixed to cut1=20 Å, are retained for the next step, the others are discarded. This has the unique goal to speed up the calculation and is legitimated by the observation that the maximal amino acid theoretical length is about 8 Å. With smaller distance cuts-off (e.g. 10 Å), some of the amino acids of the interfaces were missed.

In the second screening all the atoms of the amino acids previously retained are examined and the pairs at distance lower than cut2=5 Å are kept to form the so-called *raw interface*. This 5 Å distance covers the range of distances that corresponds to weak chemical bonds involved in interfaces: Van der

Waals, electrostatics, hydrogen bonds. Notice that these cut-offs can be freely modified. The presence of the second cut-off makes the raw interface de facto independent of the first one: values of cut1 of 17, 20, 25 Å and higher give identical results.

The raw interface is a long list of pairs of atoms that may form chemical bonds. For example, the interface of the heptamer co-chaperon 10, produced by *Mycobacter tuberculosis* (PDB code: 1HX5), has 328 pairs of atoms selected in the raw interface. Because the aim of GeminiDistances is to propose a framework with a minimum of interactions, it is necessary to add another constraint to deselect a maximum number of pairs. The deselection is performed by a *symmetrization* procedure which only retains a single interaction per atom, the one involving the closest partner, even for atoms having more than one partner on the adjacent chain. Precisely, for each atom of M, in the raw interface, only the closest atom on M+1 is retained, yielding a set of pairs $L1$. Similarly, for each atom of M+1, in the raw interface, only the closest one on M is retained to form a second set of pairs $L2$. The pairs common to both lists, $L1 \cap L2$, form the interface used for the investigations of this paper, also called *symmetrized interface*. In other words, a pair of atoms (i, j) is in the interface if both i is the closest to j and j is the closest to i .

The symmetrization makes the symmetrized interface almost cut-off independent. Indeed, values in the range cut2=4.5 to 6 Å have been explored. In the former case, some interactions are lost and the raw interface forms a subset of the raw interface obtained with cut2=5 Å. Vice versa, in the latter case the raw interface is bigger. After symmetrization, one observes remarkably small variations: in average, they do not exceed 10% of the interface in the indicated range for cut2. Variations are even smaller if only amino acids and not atoms are considered.

It is important to keep in mind that the symmetrization discards many atoms at distances for which a chemical interaction is plausible. Therefore, the output generated by GeminiDistances may miss atoms, that will be called *false negative*. It may also select atoms which are not chemically the most plausible, indicated as *false positive*. But the selection of the most chemically plausible interactions is a more difficult task than the geometrical selection performed by GeminiDistances. A more chemical selection would be necessarily slower and might not necessarily be more accurate. Such a method may be better for a case-to-case study, but the symmetrization is more appropriate for comparing the interfaces of many oligomers.

For example, from the 328 pairs of atoms selected for the raw interface of 1HX5, only 18 pairs remain after symmetrization. In a more coarse grained interpretation, the atoms of the symmetrized interface are replaced by the amino acids they belong to. This *amino acids interface* is used by the next program GeminiRegions.

GeminiDistances is written in C and runs in less than 0.2 s for an average size protein, on a normal desktop computer.

6.1.2 GeminiRegions, GeminiGraph

This program separates the amino acids interface, given by GeminiDistances, into regions, understood as elementary interaction networks between the amino acids of two adjacent chains. Many criteria can be used: the one adopted so far considers that amino acids in a region must be “close” along the sequence, in addition to be close in space as considered in the construction of the interface itself. Another interesting criterion that is implemented in Gemini is based on connected components in graph theory. According to it, atoms are grouped if there are paths that connect them by steps shorter than a given distance. This criterion ignores the sequential nature of the proteins.

This C++ program runs in the infinitesimal time of 2 ms per protein.

By construction, a region, or an interaction network, contains the interactions expressed by the pairs of the amino acids that form the interface; this corresponds to the notion of graph. In mathematics, a graph is a set of vertices (here the amino acids) connected by a set of links (here the weak chemical bonds). Therefore, it is natural to introduce the following graphical representation, done with the program

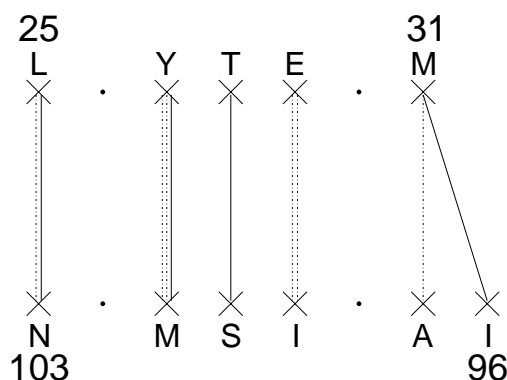


Figure 6.1. The largest region of the pentamer 1EFI (subunit B of the heat-labile enterotoxin of *Escherichia coli*) is represented here. The ladder structure formed by backbone-backbone interactions is present in most of the interfaces formed by the alignment of two parallel or antiparallel β strands.

GeminiGraph. Vertices are the amino acids; for reader's ease, those involved in a weak chemical bond are symbolised by a cross "×" whereas those not involved in weak chemical bonds are symbolized by a dot ".". Dashed-dotted lines indicate backbone-backbone interactions, solid lines indicate side chain-backbone or side chain-side chain. Amino acid type and number are indicated. See Figures 6.1, 6.2.

The interaction networks have been extensively compared with known cases in literature, observing a good assessment of the amino acids involved in protein interfaces. The comparison shows that Gemini detects rather accurately the amino acids geometrically and chemically involved in the interfaces. The chemical accuracy is particularly remarkable since the GeminiDistances selection is based on the geometry of the interface and no chemical selection is done. This recalls Crick's concept that he formulated observing α -coiled coil interfaces: the analysis of the geometry of a protein interface leads to its chemical specificity [16].

6.2 Developments

There are basically three lines of development that emerge from the Gemini interaction networks. I will briefly present them.

Firstly, the interaction networks must be analysed and systematically compared, looking for patterns. Many parameters can matter. The polarity of the residues has been preliminarily studied in [19]. Some statistics on the length of the side chain and the differential use of the amino acids has been presented in [17] and, previously, in [20]. This research continues with the main focus on the interfaces formed by the alignment of two parallel or antiparallel β strands. Nearly 60 representatives have been collected for this geometry that I will call 2β . Indeed, the ladder structure of Figure 6.1 is extremely frequently observed in this type of interface but is not observed in other interface geometries, thus it is a candidate to be a distinctive feature. This is a good example of the patterns that I would like to trace in the Gemini graphs: features that allow to distinguish geometries and to characterize their chemical properties. The preliminary analyses cited indicate that the amino acids are "flexible", they adapt to play different roles; this suggests that specific features will not be at the amino acid level but possibly to the lower level of atomic groups in the side chain. Moreover, the investigations point toward the joined structure, in which both the sides of an interface are important. Patterns or elementary blocks must appear in an interface, not just in a sequence.

Secondly, interaction networks can be used to propose amino acid substitution and test the effects with in vitro experiments. Moreover, the principles itself that I have adopted in designing the Gemini

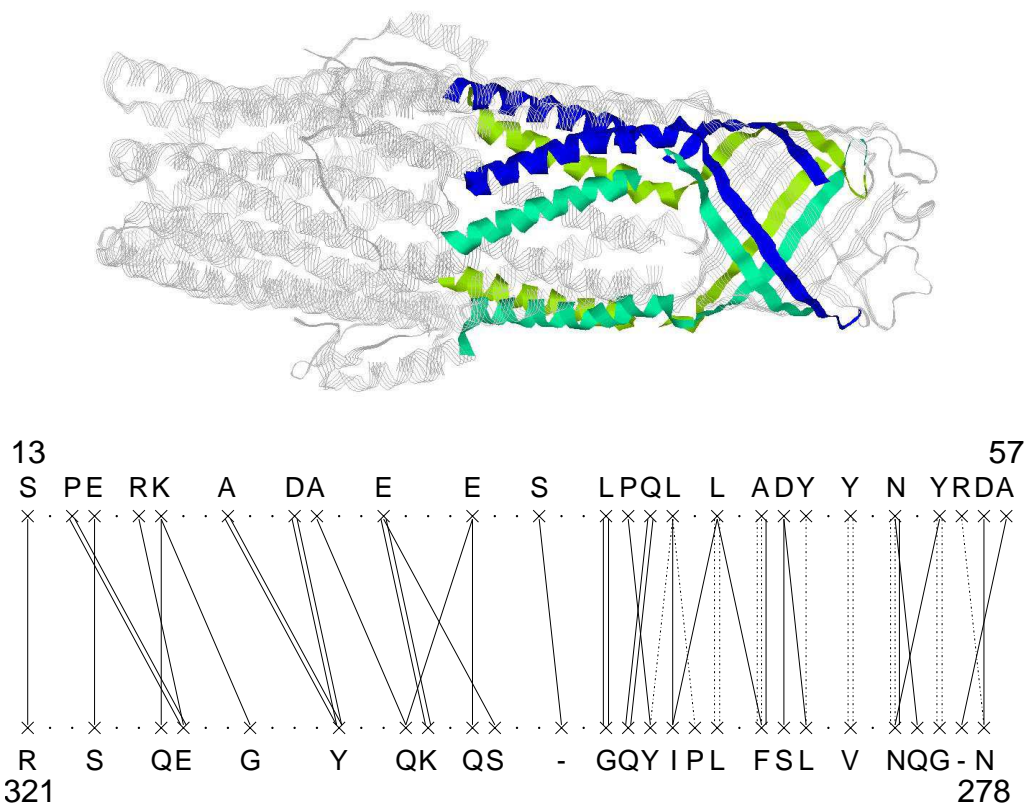


Figure 6.2. The top image enlights the α and β structures of the interface of the trimeric membrane protein TolC (PDB: 1EK9) of Escherichia coli. The bottom image contains the Gemini graph of the interface. The right part shows the same ladder structure of Figure 6.1; the left part instead is characterized by more separated amino acids, with a distance along the sequence that oscillates between 3 and 4 residues, and the presence of structures like the letter “V”, with angular separation of 3-4 residues. Indeed, this left part is an interface formed by two α -helices. Actually, it is a big α -coiled coil interface of 12 α -helices winded up in a big helix.

programs can be tested against these experiments. Given a network of interactions, it is reasonable to expect that the effect of a mutation will be different according to which amino acid is modified. In particular, little effect is expected on amino acids marked by a dot, big effect is expected for amino acids with many connections. The experimental part is of pertinence of C. Lesieur and is performed at the facilities of the BioPark of Archamps. One indication that has been found is that some interfaces are “active” even in the absence of the rest of the chain. This means that the subunits can recognize each other even when the rest of the chain has been removed. An opposite result would have indicated that the whole chain is always needed for the assembly, thus showing a marginal role of the interface.

Thirdly, one can imagine to simulate the process of association of two subunits. For this, a software is available, Simulation of Diffusional Association SDA [21]. This software implements the Langevin equation for Brownian motion and allows to trace Brownian trajectories of two molecules in water. Statistics on the trajectories produces the association rates, namely the number of encounters per time, and the residence time. Clearly, these simulations can replace in vitro experiments of association. The interest, for the Gemini team researches, is to test artificially created interfaces and study their interactions. My student J. Zrimi has invested his internship in simulating the association of different subunits of three proteins [18, 22], leading to the confirmation of a role of the four histidine in the association of these proteins.

I am directly involved in the first and third of these projects, the second being based on experimental manipulations.

6.3 Discussion

The Annecy team groups the competences and the facilities to work on both the theoretical and the experimental aspects of protein assembly, to understand the mechanisms of assembly, the sequence-structure-interface relationship, and the structural determinants of the interface geometry. I have created the team and I am the main responsible of the theoretical part. The most important result has been the creation of the programs Gemini [12], of which I am the main author (80%). For the graphical part, I asked the collaboration of my internship student [23]. The creation of these program was, more than just writing lines of code, the search of the correct ideas to translate a three-dimensional all atoms information into a synthetic description of the most relevant interactions. This process lasted for more than one year. Of course, the principles implemented in Gemini have been largely discussed with C. Lesieur and also with L. Vuillon. I have tutored several internship students. In particular, J. Zrimi has been here for a five months internship. He was student of Master 2 at the Master “Production et Valorisation des Substances Naturelles et Biopolymères” of the Faculty of sciences and techniques of Marrakech. He will come again to our laboratory for his PhD studies.

A very important event, of which I am promoter and co-organizer, is the conference “Theoretical approaches for the genome and the proteins”, TAGp2010, that will take place in Annecy-Le-Vieux in October 2010. This conference follows two previous meetings, 2008, 2006, that were focused on the genome.

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Part III

Personal research activities and publications

My publications

Referred publications

1. G. Feverati, E. Quattrini and F. Ravanini: *Infrared behaviour of massless integrable flows entering the minimal models from $\Phi_{(3,1)}$* , Phys. Lett. **B374** (1996) 64–70, hep-th/9512104, 7 pages.

Abstract. It is known that any minimal model M_p receives along its $\phi_{3,1}$ irrelevant direction two massless integrable flows: one from M_{p+1} perturbed by $\phi_{1,3}$, the other from Z_{p-1} parafermionic model perturbed by its generating parafermion field. By comparing Thermodynamic Bethe Ansatz data and “predictions” of infrared Conformal Perturbation Theory, we show that these two flows are received by M_p with opposite coupling constants of the $\phi_{3,1}$ irrelevant perturbation. Some comments on the massless S-matrices of these flows are added.

2. G. Feverati, F. Ravanini and G. Takács: *Truncated Conformal Space at $c=1$, Nonlinear integral equation and quantization rules for multi-soliton states*, Phys. Lett. **B430** (1998) 264–273, hep-th/9803104, 10 pages.

Abstract. We develop truncated conformal space (TCS) technique for perturbations of $c = 1$ conformal field theories. We use it to give the first numerical evidence of the validity of the non-linear integral equation (NLIE) derived from light-cone lattice regularization at intermediate scales. A controversy on the quantization of Bethe states is solved by this numerical comparison and by using the locality principle at the ultraviolet fixed point. It turns out that the correct quantization for pure hole states is the one with half-integer quantum numbers originally proposed by Fioravanti et al. [Phys. Lett. B 390 (1997) 243]. Once the correct rule is imposed, the agreement between TCS and NLIE for pure hole states turns out to be impressive.

3. G. Feverati, F. Ravanini and G. Takács: *Nonlinear integral equation and finite volume spectrum of sine-Gordon theory*, Nucl. Phys. **B540** (1999) 543–586, hep-th/9805117, 44 pages.

Abstract. We examine the connection between the nonlinear integral equation (NLIE) derived from light-cone lattice and sine-Gordon quantum field theory, considered as a perturbed $c = 1$ conformal field theory. After clarifying some delicate points of the NLIE deduction from the lattice, we compare both analytic and numerical predictions of the NLIE to previously known results in sine-Gordon theory. To provide the basis for the numerical comparison we use data from Truncated Conformal Space method. Together with results from analysis of infrared and ultraviolet asymptotics, we find evidence that it is necessary to change the rule of quantization proposed by Destri and de Vega to a new one which includes as a special case that of Fioravanti et al. This way we find strong evidence for the validity of the NLIE as a description of the finite size effects of sine-Gordon theory.

4. G. Feverati, F. Ravanini and G. Takács: *Scaling functions in the odd charge sector of sine-Gordon/massive Thirring theory*, Phys. Lett. **B444** (1998) 442–450, hep-th/9807160, 9 pages.

Abstract. A non-linear integral equation (NLIE) governing the finite size effects of excited states of even topological charge in the sine-Gordon (sG) / massive Thirring (mTh) field theory, deducible from a light-cone lattice formulation of the model, has been known for some time. In this letter we conjecture an extension of this NLIE to states with odd topological charge, thus completing the spectrum of the theory. The scaling functions obtained as solutions to our conjectured NLIE are compared successfully with Truncated Conformal Space data and the construction is shown to be compatible with all other facts known about the local Hilbert spaces of sG and mTh models. With the present results we have achieved a full control over the finite size behaviour of energy levels of sG/mTh theory.

5. G. Feverati, F. Ravanini and G. Takács: *Nonlinear integral equation and finite volume spectrum of minimal models perturbed by $\Phi_{(1,3)}$* , Nucl. Phys. **B570** (2000) 615–643, hep-th/9909031, 29 pages.

Abstract. We describe an extension of the nonlinear integral equation (NLIE) method to Virasoro minimal models perturbed by the relevant operator $\Phi_{(1,3)}$. Along the way, we also complete our previous studies of the finite volume spectrum of sine-Gordon theory by considering the attractive regime and more specifically, breather states. For the minimal models, we examine the states with zero topological charge in detail, and give numerical comparison to TBA and TCS results. We think that the evidence presented strongly supports the validity of the NLIE description of perturbed minimal models.

6. G. Feverati, P. A. Pearce, F. Ravanini: *Lattice approach to excited TBA boundary flows: tricritical Ising model*, Phys. Lett. **B534** (2002) 216–223, hep-th/0202041, 8 pages.

Abstract. We show how a lattice approach can be used to derive Thermodynamic Bethe Ansatz (TBA) equations describing all excitations for boundary flows. The method is illustrated for a prototypical flow of the tricritical Ising model by considering the continuum scaling limit of the A_4 lattice model with integrable boundaries. Fixing the bulk weights to their critical values, the integrable boundary weights admit two boundary fields ξ and η which play the role of the perturbing boundary fields $\varphi_{1,3}$ and $\varphi_{1,2}$ inducing the renormalization group flow between boundary fixed points. The excitations are completely classified in terms of (m, n) systems and quantum numbers but the string content changes by certain mechanisms along the flow. For our prototypical example, we identify these mechanisms and the induced map between the relevant finitized Virasoro characters. We also solve the boundary TBA equations numerically to determine the flows for the leading excitations.

7. G. Feverati, P. A. Pearce: *Critical RSOS and minimal models: fermionic paths, Virasoro algebra and fields*, Nucl. Phys. **B663** (2003) 409–442, 34 pages, enlarged version and examples in hep-th/0211185, hep-th/0211186.

Abstract. A framework is presented to extend the finitized characters and recursion methods of (off-critical) Corner Transfer Matrices (CTMs), in a self-consistent fashion, to the calculation of CFT characters and conformal partition functions. More specifically, in this paper we consider $sl(2)$ minimal conformal field theories on a cylinder from a lattice perspective. We argue that a general energy-preserving bijection exists between the one-dimensional configuration paths of the A_L Restricted Solid-on-Solid (RSOS) lattice models and the eigenstates of their double row transfer matrices and exhibit this bijection

for the critical and tricritical Ising models in the vacuum sector. To each allowed one-dimensional configuration path we associate a physical state and a monomial in a finite fermionic algebra. The orthonormal states produced by the action of these monomials on the primary states $|h\rangle$ generate finite Virasoro modules with dimensions given by the finitized Virasoro characters $\chi_h^{(N)}(q)$. These finitized characters are the generating functions for the double row transfer matrix spectra of the critical RSOS models. We also propose a general level-by-level algorithm to build matrix representations of the Virasoro generators and chiral vertex operators (CVOs). The algorithm employs a distinguished basis which we call the L_1 -basis. Our results extend to \mathbb{Z}_{L-1} parafermion models by duality.

8. G. Feverati, P. A. Pearce, F. Ravanini: *Exact $\varphi_{1,3}$ boundary flows in the tricritical Ising model*, Nucl. Phys. **B675** (2003) 469–515, hep-th/0308075, 47 pages.

Abstract. We consider the tricritical Ising model on a strip or cylinder under the integrable perturbation by the thermal $\varphi_{1,3}$ boundary field. This perturbation induces five distinct renormalization group (RG) flows between Cardy type boundary conditions labelled by the Kac labels (r, s) . We study these boundary RG flows in detail for all excitations. Exact Thermodynamic Bethe Ansatz (TBA) equations are derived using the lattice approach by considering the continuum scaling limit of the A_4 lattice model with integrable boundary conditions. Fixing the bulk weights to their critical values, the integrable boundary weights admit a thermodynamic boundary field ξ which induces the flow and, in the continuum scaling limit, plays the role of the perturbing boundary field $\varphi_{1,3}$. The excitations are completely classified, in terms of string content, by (m, n) systems and quantum numbers but the string content changes by either two or three well-defined mechanisms along the flow. We identify these mechanisms and obtain the induced maps between the relevant finitized Virasoro characters. We also solve the TBA equations numerically to determine the boundary flows for the leading excitations.

9. G. Feverati: *Exact $(d) \mapsto (+)\&(-)$ boundary flow in the tricritical Ising model*, Journal of Statistical Mechanics, J. Stat. Mech. (2004) P03001, 17 pages.

Abstract. The integrable perturbation of the degenerate boundary condition (d) by the $\varphi_{1,3}$ boundary field generates a renormalization group flow down to the superposition of Cardy boundary states $(+)\&(-)$. Exact Thermodynamic Bethe Ansatz (TBA) equations for all the excited states are derived here extending the results of [56] to this case. As an intermediate step, the non-Cardy boundary conformal sector $(+)\&(-)$ is also described as the scaling limit of an A_4 lattice model with appropriate integrable boundary conditions and produces the first example of superposition of finitized Virasoro characters.

10. G. Feverati, P. Grinza: *Integrals of motion from TBA and lattice-conformal dictionary*, Nucl. Phys. **B702** (2004) 495–515, hep-th/0405110, 21 pages.

Abstract. The integrals of motion of the tricritical Ising model are obtained by Thermodynamic Bethe Ansatz (TBA) equations derived from the A_4 integrable lattice model. They are compared with those given by the conformal field theory leading to a unique one-to-one lattice-conformal correspondence. They can also be followed along the renormalization group flows generated by the action of the boundary field $\varphi_{1,3}$ on conformal boundary conditions in close analogy to the usual TBA description of energies.

11. G. Feverati, D. Fioravanti, P. Grinza, M. Rossi, *On the finite size corrections of anti-ferromagnetic anomalous dimensions in $\mathcal{N} = 4$ SYM*, JHEP **0605** (2006) 068, hep-th/0602189, 35 pages.

Abstract. Non-linear integral equations derived from Bethe Ansatz are used to evaluate finite size corrections to the highest (i.e. *anti-ferromagnetic*) and immediately lower anomalous dimensions of scalar operators in $\mathcal{N} = 4$ SYM. In specific, multi-loop corrections are computed in the $SU(2)$ operator subspace, whereas in the general $SO(6)$ case only one loop calculations have been finalised. In these cases, the leading finite size corrections are given by means of explicit formulæ and compared with the exact numerical evaluation. In addition, the method here proposed is quite general and especially suitable for numerical evaluations.

12. G. Feverati, D. Fioravanti, P. Grinza, M. Rossi, *Hubbard's adventures in $\mathcal{N} = 4$ SYM-land? Some non-perturbative considerations on finite length operators*, J. Stat. Mech. (2007) P001, hep-th/0611186, 33 pages.

Abstract. As the Hubbard energy at half filling is believed to reproduce at strong coupling (part of) the all loop expansion of the dimensions in the $SU(2)$ sector of the planar $\mathcal{N} = 4$ SYM, we compute an exact non-perturbative expression for it. For this aim, we use the effective and well-known idea in 2D statistical field theory to convert the Bethe Ansatz equations into two coupled non-linear integral equations (NLIEs). We focus our attention on the highest anomalous dimension for fixed bare dimension or length, L , analysing the many advantages of this method for extracting exact behaviours varying the length and the 't Hooft coupling, λ . For instance, we will show that the large L (asymptotic) expansion is exactly reproduced by its analogue in the BDS Bethe Ansatz, though the exact expression clearly differs from the BDS one (by non-analytic terms). Performing the limits on L and λ in different orders is also under strict control. Eventually, the precision of numerical integration of the NLIEs is as much impressive as in other easier-looking theories.

13. J. Drummond, G. Feverati, L. Frappat and E. Ragoucy, *Super-Hubbard models and applications*, JHEP **0705** (2007) 008, hep-th/0703078, 25 pages.

Abstract. We construct XX- and Hubbard- like models based on unitary superalgebras $gl(N|M)$ generalising Shastry's and Maassarani's approach of the algebraic case. We introduce the R-matrix of the $gl(N|M)$ XX model and that of the Hubbard model defined by coupling two independent XX models. In both cases, we show that the R-matrices satisfy the Yang-Baxter equation, we derive the corresponding local Hamiltonian in the transfer matrix formalism and we determine the symmetry of the Hamiltonian. Explicit examples are worked out. In the cases of the $gl(1|2)$ and $gl(2|2)$ Hubbard models, a perturbative calculation at two loops *à la* Klein and Seitz is performed.

14. G. Feverati, K. Graham, P. Pearce, G. Tóth, G.M.T. Watts: *A renormalisation group for TCSA*, J. Stat. Mech. (2008) P03011, hep-th/0612203, 11 pag.

Abstract. We discuss the errors introduced by level truncation in the study of boundary renormalization group (RG) flows using the truncated conformal space approach (TCSA). We show that the TCSA results can have the qualitative form of a sequence of RG flows between different conformal boundary conditions. In the case of a perturbation by the field $\phi_{(1,3)}$, we propose a RG equation for the coupling constant which predicts a fixed point at a finite value of the TCSA coupling constant and we compare the predictions with data obtained using thermodynamic Bethe ansatz equations.

15. G. Feverati, F. Musso: *Evolutionary model with Turing machines*, Phys. Rev. E **77** (2008), 061901, arXiv:0711.3580, 13 pag.

Abstract. The development of a large non-coding fraction in eukaryotic DNA and the phenomenon of the code-bloat in the field of evolutionary computations show a striking similarity. This seems to suggest that (in the presence of mechanisms of code growth) the evolution of a complex code can't be attained without maintaining a large inactive fraction. To test this hypothesis we performed computer simulations of an evolutionary toy model for Turing machines, studying the relations among fitness and coding/non-coding ratio while varying mutation and code growth rates. The results suggest that, in our model, having a large reservoir of non-coding states constitutes a great (long term) evolutionary advantage.

16. G. Feverati, L. Frappat and E. Ragoucy, *Universal Hubbard models*, J. Stat. Mech. (2009) P04014, arXiv:0903.0190, 34 pag.

Abstract. We propose a general framework that leads to one-dimensional XX and Hubbard models in full generality, based on the decomposition of an arbitrary vector space (possibly infinite dimensional) into a direct sum of two subspaces, the two corresponding orthogonal projectors allowing one to define a R -matrix of a universal XX model, and then of a Hubbard model using a Shastry type construction. The QISM approach ensures integrability of the models, the properties of the obtained R -matrices leading to local Hubbard-like Hamiltonians.

17. F. Musso, G. Feverati: *A proposal for an optimal mutation probability in an evolutionary model based on Turing machines*, in Intelligent Data Engineering and Automated Learning - IDEAL 2009 (E. Corchado, H. Yin Editors), Lectures Notes in Computer Sciences (LNCS) 5788 Springer, pp.735-742 (2009), LAPTH-1332/09. Referred proceedings of the 10th IDEAL International Conference, Burgos, Spain, 23-26 September 2009.

Abstract. In our previous paper we defined an evolutionary computation model based on Turing Machines. One of the aims of the paper was to determine empirically the optimal mutation and states-increase rates. After, we made some changes in our model and we run some of the previous simulations for larger values of the states-increase rate. Moreover we performed a mathematical analysis of our model. Such analysis suggests an adaptative expression for the optimal mutation probability. We run new simulations with such a choice of mutation probability and with the maximum states-increase rate attained. We compare the results of this simulations with our previous ones relative to the empirical optimal constant mutation probability with the same states-increase rate.

18. G. Feverati, P. A. Pearce and N. S. Witte: *Physical combinatorics and quasi-particles*, J. Stat. Mech. (2009), P10013, arXiv:0903.0510, LAPTH-1293/08, 54 pag.

Abstract. We consider the physical combinatorics of critical lattice models and their associated conformal field theories arising in the continuum scaling limit. As examples, we consider A -type unitary minimal models and the level-1 $sl(2)$ Wess-Zumino-Witten (WZW) model. The Hamiltonian of the WZW model is the $U_q(sl(2))$ invariant XXX quantum spin chain. For simplicity, we consider these theories only in their vacuum sectors on the strip. Combinatorially, fermionic particles are introduced as certain features of RSOS paths. They are composites of dual-particles and exhibit the properties of quasi-particles. The particles and dual-particles are identified, through a conjectured energy preserving bijection, with patterns of zeros of the eigenvalues of the fused transfer matrices in their analyticity strips. The associated (m, n) systems arise as geometric packing constraints on the particles. The analyticity encoded in the patterns of zeros is the key

to the analytic calculation of the excitation energies through the Thermodynamic Bethe Ansatz (TBA). As a by-product of our study, in the case of the WZW or XXX model, we find a relation between the location of the Bethe root strings and the location of the transfer matrix 2-strings.

19. G. Feverati, C. Lesieur: *Oligomeric interfaces under the lens: Gemini*, PLoS ONE 5(3): e9897 (2010), LAPTH-1349/09, 15 pag.

Abstract. The assembly of subunits in protein oligomers is an important topic to study as a vast number of proteins exists as stable or transient oligomer and because it is a mechanism used by some protein oligomers for killing cells (e.g., perforin from the human immune system, pore-forming toxins from bacteria, phage, amoeba, protein misfolding diseases, etc.). Only a few of the amino acids that constitute a protein oligomer seem to regulate the capacity of the protein to assemble (to form interfaces), and some of these amino acids are localized at the interfaces that link the different chains. The identification of the residues of these interfaces is rather difficult. We have developed a series of programs, under the common name of Gemini, that can select the subset of the residues that is involved in the interfaces of a protein oligomer of known atomic structure, and generate a 2D interaction network (or graph) of the subset. The graphs generated for several oligomers demonstrate the accuracy of the selection of subsets that are involved in the geometrical and the chemical properties of interfaces. The results of the Gemini programs are in good agreement with those of similar programs with an advantage that Gemini programs can perform the residue selection much more rapidly. Moreover, Gemini programs can also perform on a single protein oligomer without the need of comparison partners. The graphs are extremely useful for comparative studies that would help in addressing questions not only on the sequence specificity of protein interfaces but also on the mechanism of the assembly of unrelated protein oligomers.

20. A. Doikou, S. Evangelisti, G. Feverati, N. Karaiskos: *Introduction to quantum integrability*, Lecture notes given at the Università di Bologna in 2007 by A.D. and G.F. and at the Università di Patras in 2009 by A.D.; the edition has been done in collaboration with the students S.E. and N.K.; published on Int. J. Mod. Phys. 25 (2010) 3307-3351, arXiv:0912.3350, LAPTH-1367/09, 56 pag.

Abstract. In this article we review the basic concepts regarding quantum integrability. Special emphasis is given on the algebraic content of integrable models. The associated algebras are essentially described by the Yang-Baxter and boundary Yang-Baxter equations depending on the choice of boundary conditions. The relation between the aforementioned equations and the braid group is briefly discussed. A short review on quantum groups as well as the quantum inverse scattering method (algebraic Bethe ansatz) is also presented.

21. J. Zrimi, A. Ng Ling, E. Giri-Rachman Arifin, G. Feverati, C. Lesieur, *Cholera toxin B subunits assemble into pentamers: proposition of a fly-casting mechanism*, 2010, accepted by Plos One.

Abstract. The cholera toxin B pentamer (CtxB5), which belongs to the AB5 toxin family, is used as a model study for protein assembly. The effect of the pH on the reassembly of the toxin was investigated using immunochemical, electrophoretic and spectroscopic methods. Three pH-dependant steps were identified during the toxin reassembly: (i) acquisition of a fully assembly-competent fold by the CtxB monomer, (ii) association of CtxB monomer into oligomers (iii) acquisition of the native fold by the CtxB pentamer. The results show that CtxB5 and the related heat labile enterotoxin LTxB5 have distinct mechanisms of assembly despite sharing high sequence identity (84%) and almost identical atomic structures. Subtle differences in the two toxins amino acid compositions are

therefore responsible for the different folding and assembly pathways followed by the two closely related toxins. In particular, histidine residues appear to be good candidates to explain the two toxin different mechanisms of assembly.

Code protection

DP 1. G. Feverati: *Gemini*, ensemble of programs (GeminiDistances, GeminiRegions, GeminiGraph), registered at the Agence pour la protection des programmes (APP), DI 3330-01. ¹

Proceedings of conferences

A 1. G. Feverati, P. A. Pearce and F. Ravanini: *Excited boundary TBA in the tricritical Ising model*, talk given by F. Ravanini at the Landau Workshop *CFT and Integrable Models*, Chernogolovka (Moscow), Sept. 2002, arXiv:hep-th/0306196, Int. J. Mod. Phys. **A19**, Supplementary Issue 2 (2004) 155, 13 pages.

Abstract. By considering the continuum scaling limit of the A_4 RSOS lattice model of Andrews-Baxter-Forrester with integrable boundaries, we derive excited state TBA equations describing the boundary flows of the tricritical Ising model. Fixing the bulk weights to their critical values, the integrable boundary weights admit a parameter ξ which plays the role of the perturbing boundary field $\varphi_{1,3}$ and induces the renormalization group flow between boundary fixed points. The boundary TBA equations determining the RG flows are derived in the $\mathcal{B}_{(1,2)} \rightarrow \mathcal{B}_{(2,1)}$ example. The induced map between distinct Virasoro characters of the theory are specified in terms of distribution of zeros of the double row transfer matrix.

A 2. J. Drummond, G. Feverati, L. Frappat, E. Ragoucy: *Generalised integrable Hubbard models*, talk given by G. Feverati at the workshop *RAQIS'07 Recent Advances in Quantum Integrable Systems*, LAPTH, Annecy-le-Vieux, France, 11-14 September 2007, arXiv:0712.1940, 15 pages. Edited and printed by L. Frappat and E. Ragoucy.

Abstract. We construct the XX and Hubbard-like models based on unitary superalgebras $gl(N|M)$ generalizing Shastry's and Maassarani's approach.

We introduce the R-matrix of the $gl(N|M)$ XX-type model; the one of the Hubbard-like model is defined by "coupling" two independent XX models. In both cases, we show that the R-matrices satisfy the Yang-Baxter equation. We derive the corresponding local Hamiltonian in the transfer matrix formalism and we determine its symmetries.

A perturbative calculation "à la Klein and Seitz" is performed. Some explicit examples are worked out. We give a description of the two-particle scattering.

Posters

P 1. F. Musso, G. Feverati: *An evolutionary model for Turing machines*, presented by F. M. at the workshop *Theoretical Approaches for the Genome*, 8-10 November 2006, LAPTH Annecy, France.

P 2. G. Feverati, L. Vuillon, P. Sorba, C. Lesieur: *Protein oligomeric interfaces: a tool to address the protein assembly issue*, presented by C.L. at the workshop *Protein evolution: sequences, structures and systems*, Cambridge, Jan. 2009.

¹The registration of a computer program is regulated by the laws of authorship and gives a protection equivalent to the one obtained with a patent. The European laws exclude the possibility to patent computer programs.

Other writings

- T 1. G. Feverati: *Matrici S in teorie quantistiche di campo integrabili non massive a 1+1 dimensioni*, (*S matrices in 1+1 dimensional integrable massless quantum field theories*), Master thesis, in italian, 1995, 96 pag., unpublished.

Abstract. This text presents the factorized scattering theory for two-dimensional integrable theories, the Zamolodchikov thermodynamic Bethe ansatz method for the ground state and few integrable theories where a massless scattering occurs. Particularly, the S-matrix of the deformed $O(3)$ σ -model (“sausage” model) is discussed.

- T 2. G. Feverati: *Finite Volume Spectrum of Sine-Gordon Model and its Restrictions*, PhD thesis, 1999, hep-th/0001172, 96 pag.

Abstract. In this thesis, we review recent progresses on Nonlinear Integral Equation approach to finite size effects in two dimensional integrable quantum field theory, with emphasis to Sine-Gordon/Massive Thirring model and restrictions to minimal models perturbed by $\Phi_{1,3}$. Exact calculations of the dependence of energy levels on the size are presented for vacuum and many excited states.

Preprints

- Pre. 1. F. Musso, G. Feverati, *Mutation-Selection Dynamics and Error Threshold in an Evolutionary Model for Turing Machines*, (2010) submitted to Plos One.

Abstract. We investigate the mutation-selection dynamics for an evolutionary computation model based on Turing Machines that we introduced in a previous article.

The use of Turing Machines allows for very simple mechanisms of code growth and code activation/inactivation through point mutations. To any value of the point mutation probability corresponds a maximum amount of active code that can be maintained by selection and the Turing machines that reach it are said to be at the error threshold. Simulations with our model show that the Turing machines population evolve towards the error threshold.

Mathematical descriptions of the model point out that this behaviour is due more to the mutation-selection dynamics than to the intrinsic nature of the Turing machines. This indicates that this result is much more general than the model considered here and could play a role also in biological evolution.